1981

Natural Convection, Two-Phase Flow, and Crystallization in a Vacuum Pan Sugar Crystallizer.

Jack Jerome Bunton
Louisiana State University and Agricultural & Mechanical College

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The Louisiana State University and Agricultural and Mechanical Col. PH.D. 1981

NATURAL CONVECTION, TWO-PHASE FLOW, AND CRYSTALLIZATION IN A VACUUM PAN SUGAR CRYSTALLIZER

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by

Jack Jerome Bunton
B.S., University of South Alabama, 1976
M.S., Louisiana State University, 1978

May 1981

To My Daughter Brianna,

With Love

ACKNOWLEDGEMENT

Foremost, I would like to express my special gratitude to my wife Toni, whose patience, love, and understanding allowed me to complete this research.

I would like to express my appreciation to my Committee members, Drs. Lawrence Mann, Bert Wilkins, Ralph W. Pike, and Joseph Polack for their comments and suggestions based upon their review of this work. Special thanks to Armando B. Corripio and Richard C. Farmer for advice and guidance in the development of this research.

Special appreciation to Hazel LaCoste and other members of the staff of the department of Chemical Engineering, as well as, the members of the staff of the Audubon Sugar Institute for their continuing support of graduate students pursuing an advanced degree.

I am grateful for the financial assistance provided by the Audubon Sugar Institute. Also, I would like to thank the Dr. Charles E. Coates Memorial Fund, donated by Charles E. Coates, for financial aid in the preparation of this manuscript.

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ABSTRACT

A mathematical model of a Vacuum Pan Sugar Crystallizer is developed. This mathematical model is based on the fundamentals of the physics of two-phase flow. Because of the complexity of the model, the time dependent solution is accomplished using numerical methods designed to be executed by a digital computer. The model generates velocity, pressure, temperature, and supersaturation profiles for the Pan, in response to the operating conditions and the design of the Pan. The motivation for the development of this model is to give an analytical tool to study the effects of Pan design, control systems, and operating conditions on the product crystal size distribution.

The emphasis of this research is on the development of the numerical methods that are consistent with conservative and transportive principles reflected in the equations of motion. Important features of the numerical code are that it employs a dynamic grid system designed for free surface flows, and is compatible with viscous two-phase flows exhibited in the Pan. The modeling equations are two-dimensional for the volume above the Calandria, but in other areas where two-dimensional equations are an extravagance, one-dimensional and lumped equations are used.

The velocity and growth rate profiles provides the information needed for a distributed population balance equation needed to analyze the effect of these profiles on the crystal size distribution. The development of such a population balance is discussed but is not part of the present numerical code. Nonetheless, the model provides valuable information concerning the effects of Pan design, control systems, and operating conditions in a qualitative sense, as demonstrated in the results. Sensitivity studies varying Pan design and operating conditions demonstrate that of the cases studied, the volumn fraction crystals, pan level, heat load, pan pressure, and whether or not the pan major diameter is flared, had the most significant effects on the pan performance. These variations of Pan design and operating conditions were judged significant based on their effect on the velocity and growth profiles, maximum and minimum supersaturation, and average supersaturation. A summary of the results is presented in Chapter 7 and discussions concerning particular cases along with raw data are presented in Chapter 5.

CHAPTER 1

INTRODUCTION

The purpose of this research is to develop a mathematical model of the transport phenomena in a Vacuum Pan Sugar Crystallizer and to use it to study its effect on the crystal size distribution (CSD), and its control. The proper conservative equations will be found or derived, that under proper assumptions and simplifications, and when given the proper boundary conditions, will adequately describe the conditions of fluid flow in the pan. Once the proper equations have been found, further assumptions will be made to model sections of the pan where the characteristics of the flow are different.

The development of the mathematical model is based on the fundamental conservation equations of mass, momentum, and energy as applied to a multi-phase system. The phases present during the operation of the Vacuum Pan are the liquid sugar solution, solid sugar crystals, and water vapor because the mixture is boiling. The mathematical model is spatially distributed rather than lumped. The motive for development of this model is to study the effect of spatially varying growth rates on the resulting CSD. The growth variations are the result of the distributed nature of the temperature profiles in the

Vacuum Pan. Although, the purpose of this research is to develop the model describing the fluid mechanics, emphasis is placed on the use of this model to analyze the CSD. In fact, Chapter 2 is a summary of the equations used in the literature to model particulate systems such as the Vacuum Pan.

Before going any further, let's describe the Vacuum Pan with enough detail so that the reader may understand subsequent discussion in reference to the Pan. Figure 1.0.0 is the symetrical half-section of an idealized pan divided into sections that will have meaning later.

Basically, the Vacuum Pan is a Calandria type evaporator with a central downtake. The objective of the Vacuum Pan is to provide a supersaturated environment to promote crystal growth. Sugar content in the water solution is depleted by crystal growth and replenished by unsaturated liquid feed. Thus, water is evaporated continuously to maintain supersaturated conditions. Careful consideration is given to pan temperature, therefore, the pan is operated under vacuum to maintain low boiling temperature because the sugar crystals are heat sensitive. The massecuite (a sugar solution with crystalline sugar in suspension), is heated in the Calandria and the hot mixture rises as the result of density differences between the column of the mixture

above the Calandria Downtake and the column above the Calandria Heating Section. Boiling may occur as the mixture rises towards the surface. The heat generated in the Calandria is released at the surface in the form of vapor, if the boiling point of the mixture has been reached. That which has not left the pan in the form of vapor is recirculated back through the Calandria via the Downtake. Because of the highly viscous nature of the sugar solution, sugar crystals generally flow with approximately the same velocity as the surrounding fluid even though the density difference is significant. The amount of sugar in the solution remains relatively constant throughout the pan volume at any given time, but, the local solution temperature may change drastically relative to local sugar concentration changes. Thus, growth profiles result due to temperature profiles in the Pan.

Important features of the Vacuum Pan Sugar Crystallizer needed for consideration in the derivation of the mathematical model describing the fluid flow are that, the flow is by natural convection, free surface, possibly boiling, and highly viscous. However, different sections may be characterized independently and if these characteristics are capitalized upon, a more efficient numerical computor code may be formulated without neglecting the major features mentioned above. The following sections are separated as shown in

Figure 1.0.0 because of their different characteristics.

1. Pan Proper
2. Bottom and Downtake
3. Calandria
4. Free Surface

To this point, the significance of the CSD is not apparent. A narrow CSD is desirable and it is the objective of the Vacuum Pan to grow an initially uniform seed CSD to an acceptable size, dictated by the maximum volume of crystal that the mother liquor can suspend and still be reasonably fluid. The volume fraction of crystal is usually less than forty percent at the end of the batch. A wide CSD or large variance of the CSD reduces the fluidity of the mixture for a given volume fraction of crystals. This makes the separation of the crystals at the end of the batch by centrifuging difficult and also hinders circulation in the Vacuum Pan. Circulation in the Pan must be maintained to prevent further widening of the CSD.

A narrow CSD is also desirable because a wider CSD is not generally marketable as a consumer product. Of course, a narrow CSD indicates that nucleation has been avoided. Since nucleation causes crystal aggregates to be formed, which occludes mother liquor containing impurities, and noting that purity is also important, a

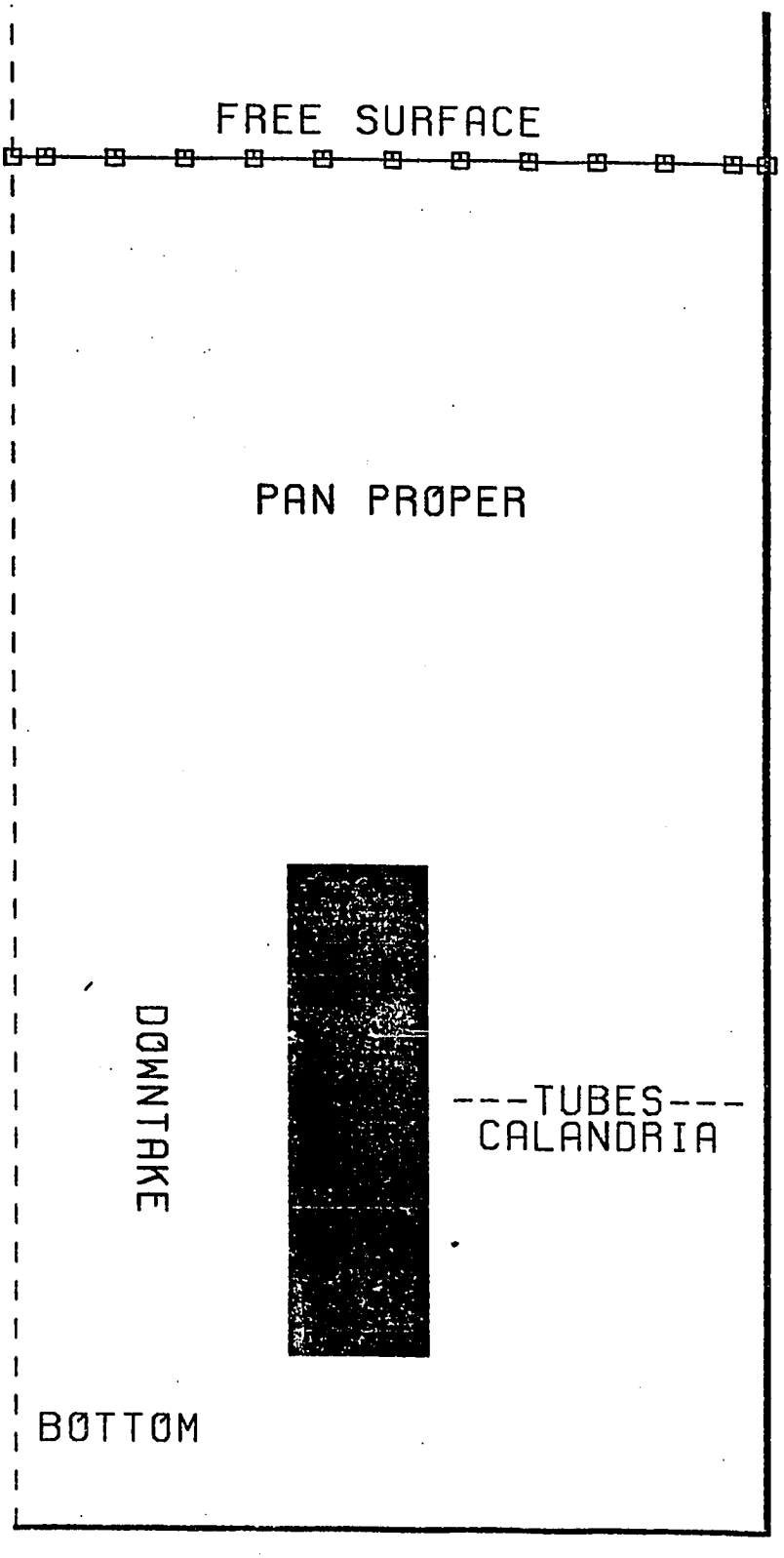


FIGURE 1.0.0 IDEALIZED VACUUM PAN

narrow CSD is desirable. Thus, a narrow CSD is important from the standpoint of the operation of the Pan, separation of the product, and from customer specifications. Therefore, a model capable of predicting the conditions that cause a widening of the CSD and studying control methods to minimize these conditions as much as possible, is desirable.

Previous work in modeling the Vacuum Pan for the purpose of simulation and control studies have been based on the Well Stirred Tank (WSTRT) principle. These models employ the basic material and energy balances as applied to the WSTRT, as well as, the basic physical properties and kinetic information as pertaining to the sucrose crystallizer. Recent advances in modeling particulate systems through the use of the particle population balance aid in the understanding of the operation of the Vacuum Pan. Wright (1974), Frew (1973), and Mukhopadhyay (1980) use these recent advances in studying particulate systems along with the overall material and energy balance to develop a mathematical model of the Vacuum Pan. Both Wright (1974) and Mukhopadhyay (1980) develop the model as a simulation tool to study the effects of certain variables. However, Mukhopadhyay (1980) considers the competing kinetics of nucleation and growth to change the CSD, while Wright (1974) ignores nucleation but includes an empirical dispersion coefficient that describes the

widening of the CSD due to mixing effects. Frew (1973), on the other hand, develops the model in order to apply optimal control theory to optimize the operation of the batch. However, Frew's conclusions are the same as might be concluded based on experience or with a little engineering insight. Earlier modeling efforts by Doucet (1966), Mori (1968), Evans (1970), and Batterham (1974) do not employ the population balances and are aimed at understanding and designing the basic material and energy balance control systems. Doucet, Evans, and Batterham develop and apply their models in the time domain, but Mori linearizes the modeling equations and places them in the Laplace domain in a more traditional control theory approach.

Although the emphasis here is on semi-continuous or the batch Vacuum Pan, Randolph (1978) and Sowal (1979) have published articles concerning continuous sucrose crystallizers and the application of the particle balances.

In the following chapters, the mathematical model of the Vacuum Pan will be developed. Although the main purpose of this research is to develop a model describing the fluid mechanics, for the sake of completeness, the population balances for spatially distributed and lumped systems will be discussed in Chapter 2. However, these balances will not be integrated into the numerical model,

instead, the crystal growth will be treated very simply for material balance purposes. The spatial dependence of the growth rate will be demonstrated with local calculation of the growth rate based on the local temperature and the pan sucrose and impurities concentrations. Extensions of this model to include the lumped or distributed particle balances will allow a direct analysis of the effects of pan design, operating conditions, and control systems on the CSD. Concluding this research, sensitivity studies will be performed to demonstrate the effects of pan design and operating conditions on the velocity profiles and growth rate profiles. These, of course, directly affect the CSD and demonstrate the usefulness of the model as a research tool. In addition to the velocity and growth rate profiles, the model also generates temperature and pressure profiles in the Pan.

Because of the system of equations describing the physics of fluid motion in the Vacuum Pan are complex, the numerical solution of these equations is particularly difficult. It is for this reason that the derivation of the applied equations, under the proper assumptions, is so important in order to facilitate the numerical solution and reduce the complexity of the numerical solution. The solution method described for the modeling equations and concepts brought out in this research are

very much at the forefront of the state of the art in computational fluid mechanics for free surface flows. Much of the emphasis of this research is therefore, placed on the development of the modeling equations and their numerical solution.

Application of the model to other problems involving a free surface is obvious, since it is based on the fundamentals of fluid mechanics. As this research is an extension of earlier research done at Louisiana State University, by Waldrop (1972) and Pitts (1976), on modeling bays and estuaries, the improvements and extensions accomplished in this research are directly applicable to these earlier codes. The code described here can be easily extended to study circulation patterns caused by hot submerged jets in bodies of water. The Oak Ridge Simplified Marker and Cell Code, developed by Park (1980), was developed to simulate such a situation, but the code developed in this research is simpler and more efficient with computer time, which are obvious advantages. In addition, the development of the dynamic grid system, which is essential when modeling free surface flows, is presented with more mathematical rigor than presented in the literature and should aid in the development of other free surface fluid dynamic codes.

CHAPTER 2

PARTICLE EQUATIONS

The analysis of particulate systems such as dryers, fluidized beds, and crystallizers, among others, has been greatly enhanced by the development of the population balances. An excellent source of discussion and application of these population balances is contained in a book by Randolph and Larson (1971).

Because the biological sciences are also interested in information concerning the ages or sizes of biological organisms, these equations apply directly to the analysis of those systems. The concise mathematical framework of this set of equations, through analytical or numerical solutions of the applied equations, allows analysts to simulate particulate systems or interpret experimental data.

As applied to crystallizers, the growth and nucleation rate of crystals may be identified from experiments or the CSD predicted. To demonstrate how kinetic data might be interpreted, the continuous Well Stirred Tank (WSTRT) crystallizer will be described mathematically with reference to Figure 2.0.0. This population balance will serve to identify the kinetics of the crystallizer or model the crystallizer. The important point, however, is that once the kinetics have

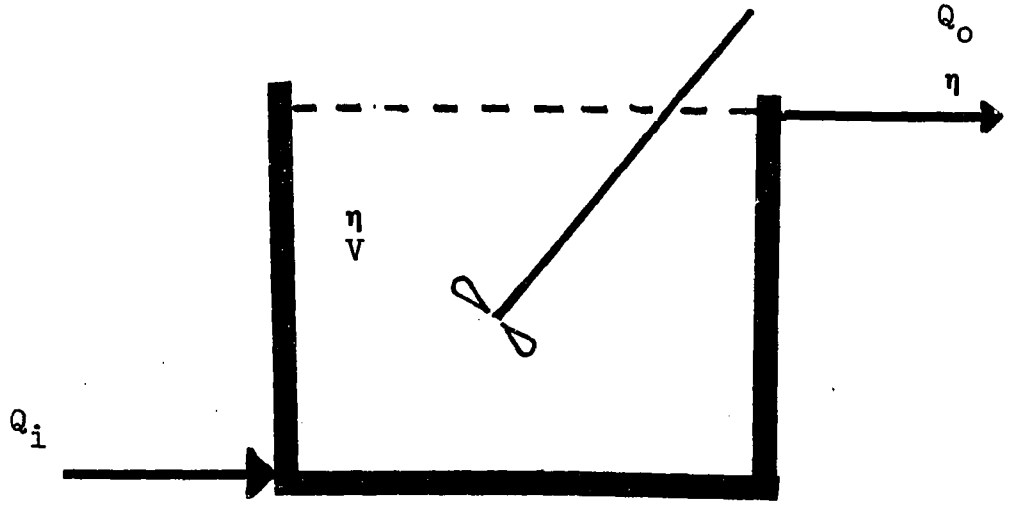


FIGURE 2.0.0 WELL STIRRED TANK CRYSTALLIZER

been identified, the population balances can be derived for more complex physical systems and hopefully, the kinetics still apply.

The population balances for the WSTRT are derived like the material and energy balances, except, the conserved quantity is the number of particles in a particular size range. The function that mathematically describes the population in question is its crystal size distribution (CSD). The function is generally approximated by a continuous function rather than a discrete function. Figure 2.0.1 is a typical CSD, that might be obtained by a sieve analysis or various other methods. Since the crystals are suspended in a volume of mother liquor, in a crystallizer, to facilitate the analysis, a new variable will be defined as the crystallizer number density, as defined by Equation 2.0.0.

$$\eta = \frac{CSD}{V} N_c \qquad 2.0.0$$

Where V is the volume of the mother liquor rather than the total volume. The number of crystals per unit volume in the crystallizer between the sizes of L to L+dL is then defined by Equation 2.0.1.

$$V\int_{L}^{L+dL} \eta \, dL = V\eta(L)dL \qquad 2.0.1$$

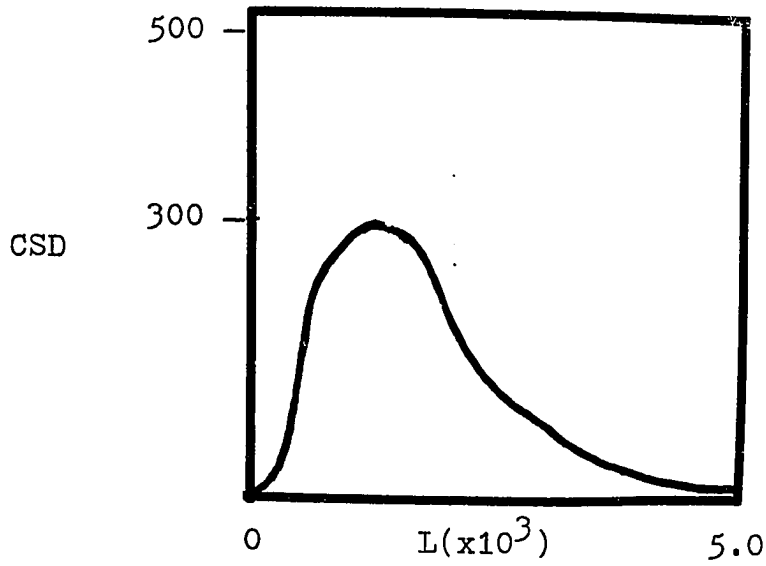


FIGURE 2.0.1 TYPICAL CRYSTAL SIZE DISTRIBUTION

The change in time of the number of crystals in the size range is the result of the birth or the nucleation rate of new crystals, the input of seed crystals with the feed, and output of crystals in the output stream, and the growth of crystals. The function which describes the rate at which nuclei are produced in all size ranges per unit volume of mother liquor, is the nucleation rate density function (NRDF), and is approximated with a continuous function (B). The mechanisms that cause nucleation and the theory behind them are discussed in Mullin (1975). For most modeling efforts the nucleation of new crystals is described mathematically as a power law function of the growth rate or supersaturation. The growth rate (G) of the crystals in the solution is generally expressed as a power law function of supersaturation. The theory of growth of crystals is also discussed in Mullin. Although, birth of crystals can be thought of as occurring in all sizes, for the purposes here, the NRDF describes the nucleation of crystals at the zero size. For this analysis, no crystals will be supplied with the feed. The population balance is expressed mathematically in Equation 2.0.2.

$$\frac{\partial (V\eta(L)dL)}{\partial t}\Delta t = -\Delta t Q_o \eta(L)dL + \Delta t V B(L)dL \qquad 2.0.2$$
$$+ V(\eta(L-G\Delta t)G\Delta t - \eta(L)G\Delta t)$$

Dividing both sides of Equation 2.0.2 by dL, Δt, and V and taking the limit as dL and Δt, go to zero, Equation 2.0.3 is the resulting equation. The domain of Equation 2.0.3 is crystal sizes greater than or equal to zero.

$$\frac{\partial \eta V}{V \partial t} = \frac{\partial \eta}{\partial t} + \frac{d \ln V}{dt} = - \frac{\eta}{V} Q_o - \frac{\partial \eta G}{\partial L} + B \qquad 2.0.3$$

Equation 2.0.3 is the population balance for the WSTRT model. However, to obtain information about the kinetics from experimental data collected from the WSTRT, Equation 2.0.3 can be simplified to allow an analytic solution. Equation 2.0.4 results from neglecting the dynamic terms. The boundary conditions for Equation 2.0.4 are given below the equation, the functionality of B is also given.

$$\begin{aligned} &\frac{d \eta G}{\partial L} = - \frac{\eta}{V} Q_o \\ &\eta(0) = \eta_o = B_o / G \\ &\eta(\infty) = 0 \\ &B(0) = B_o \\ &B(L) = 0 \quad L>0 \end{aligned} \qquad 2.0.4$$

Equation 2.0.4 applies for crystal sizes greater than zero but is made to include zero size by applying the boundary condition at the zero crystal size. This

boundary condition is derived by doing a particle balance for the zero size as given by Equation 2.0.5.

$$\frac{d\eta_o}{dt} = -\eta_o G + B_o \qquad 2.0.5$$

Therefore at steady state, the nuclei density (η_o) is simply the ratio of the nucleation rate to the growth rate. The solution to Equation 2.0.4, given the functional definition of B, the boundary conditions and growth rate not a function of the length, is given in Equation 2.0.6 below.

$$\eta = \eta_o EXP(-\frac{LQ_o}{VG}) \qquad 2.0.6$$

Therefore, by taking experimental data from a WSTRT crystallizer at a steady state, one may obtain the growth rate and nucleation rate at the conditions in the crystallizer. Then, by studying various conditions, a functional relationship may be obtained between the conditions (supersaturation, impurities, etc.) in the WSTRT and the growth and nucleation rates. The traditional method of analysis is to plot the logarithm of the crystal number density function (η) as a function of the crystal size and extract the slope and intercept,

but other mathematical techniques may be used. Figure 2.0.2 is a typical plot.

Once the kinetics of the system have been established, by experiment, one may use Equation 2.0.3 to model the dynamics of the continuous WSTRT in response to changes in operating conditions or the effect of various control systems. However, Equation 2.0.3 is too complex for analytical solution and, therefore, a numerical solution must be attempted. Since Equation 2.0.3 is a partial differential equation, the equation could be partitioned into a set of particle size ranges and intergrated as partial differential equations are traditionally treated. This is the approach Grimmett (1980) takes in studying Fluidized-Bed Dryers. However, generally speaking, the complete distribution need not be reproduced during a numerical simulation, instead, a few descriptive parameters are all that are needed, specifically, the average particle size, the total number of particles, and the variance of the CSD. Of course, all of these can be obtained from the crystallizer number density function, since it is related to the CSD via Equation 2.0.0. Thus, following the moments of the crystallizer number density function, one can follow the performance of the crystallizer. Following the moments also eliminates the problems of a partial differential equation, since the particle size dimension is integrated out when Equation 2.0.3 is

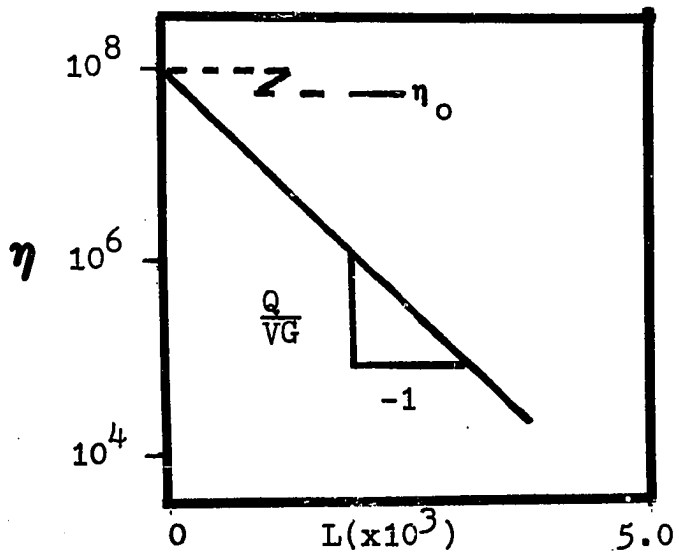


FIGURE 2.0.2 TYPICAL CRYSTAL NUMBER DENSITY FUNCTION

converted to a moment equation. This is done by the integration described in the equation below.

$$\int_0^{\infty} L^k \frac{\partial \eta}{\partial t} dL + \frac{d\ln V}{dt} \int_0^{\infty} L^k \eta dL = - Q_o/V \int_0^{\infty} L^k \eta dL$$

$$- G \int_0^{\infty} L^k \frac{\partial \eta}{\partial L} dL + \int_0^{\infty} L^k B(L) dL \qquad 2.0.7$$

$$k = 0,1,2...$$

Equation 2.0.7 can be integrated for each value of k, given the definition of the kth moment of η, Equation 2.0.8, and by using integration by parts for moments higher than zeroth moment.

$$M_k = \int_0^{\infty} L^k \eta dL \qquad k = 0,1,2... \qquad 2.0.8$$

The results of the integration are summarized below.

$$B_k = \int_0^{\infty} L^k B dL \qquad k = 0.1.2... \qquad 2.0.9$$

$$\frac{dM_k}{dt} + M_k \frac{d\ln V}{dt} = - M_k Q_o/V + kGM_{k-1} + B_k \qquad 2.0.10$$

$$M_{-1} = \eta_o \qquad 2.0.11$$

$$B_k(k=0) = B_o \qquad 2.0.12$$

$$B_k = 0 \qquad k = 1,2,3...$$

The total number of crystals in the WSTRT, the average length, and the variance of the CSD, is then related to the moments, as shown in Equation 2.0.12 thru 2.0.15.

$$N_c = M_o V \qquad 2.0.13$$

$$\bar{L} = M_1/M_o \qquad 2.0.14$$

$$\sigma^2 = M_2/M_o - (M_1/M_o)^2 \qquad 2.0.15$$

These equations can be integrated along with the overall material and energy balances and be used to study the dynamics of the WSTRT.

Although, in many cases, the WSTRT principle is adequate for most industrial applications where particulate processing is involved, there are cases where this is not true. Such a case is the semi-continuous operation of the Vacuum Pan Sugar Crystallizer. Because the sugar solution is viscous and mixing is generally caused by natural convection and boiling, growth and

supersaturation profiles exist. Crystals flowing with the fluid are, therefore, subjected to a varying growth environment which contributes to the widening of the CSD. Because supersaturation at points may be excessive, even though the average supersaturation is satisfactory, nucleation may occur which further disturbs the CSD. Analysis of this system can only be done satisfactorily when these problems are taken into account in the modeling effort. One way to model such a system is to use a distributed population balance. Hulburt and Katz (1964) develop such a distributed population balance, based on continuum principles. The development of the distributed equation considers distributed conditions to promote growth and nucleation and convection of the crystals with the fluid. Unfortunately, Hulburt and Katz developed the equations for incompressible flow only, therefore, the equations do not directly apply to the Vacuum Pan because of the boiling phenomenon. Because the use of the distributed equations requires the velocity, growth, and nucleation profiles, these equations must be combined with the distributed equations of mass, momentum, and energy. To be compatible with the fluid dynamic equations and their numerical solution, as developed in the pages to follow, additional research will be needed to construct the proper crystal size number density and the form of the

population balance. Possible alternative formulations of the distributed population balance accommadating compressible flow, might be to express the number density (η) on a per unit mass of mixture basis, to be compatible with the homogeneous flow assumption used in the development of the equations of motion in the following chapters. On a per mass basis, the population balance will have the form of the mixture momentum equation without the diffusion terms. A more physical alternative would be to consider the crystals as remaining in the liquid phase all the time, in which case, the incompressible flow assumption will be valid and the population balance will only have to be modified to include the volume fraction of liquid. Although the distributed analysis is a formidable test, analyses of this type have been attempted successfully, but not for the crystallizer. For example, Bracco (1974) analyzes the combustion of flammable liquid drops falling in hot air using the distributed population balance with fluid flow. Thus, such a modeling effort is possible and if carried out, should aid in the understanding of the operation of the Vacuum Pan and help eliminate some of the problems that cause a widening of the CSD.

CHAPTER 3

MATHEMATICAL MODEL

Over the past twenty years with the advent of fast computers, the utility of studying physical systems by numerically solving the fundamental mathematical equations describing the physical system has increased. This is the result of the high cost of failure of the designed system to meet specifications or safety requirements. For most mathematical formulations of the physical systems, analytical solutions of the set of equations are not possible, therefore, a solution must be found through the use of numerical methods. The ease of solving these equations depends on the complexity of the problem and the particular characteristics of the numerical formulation of the problem. Once a realistic and solvable mathematical model has been developed, the model can then be used to simulate the system of interest. The advantage here is that computational experiments can be performed that can optimize the systems complete design, including control systems as well as safety systems. All of this can be done before large expenditures are wasted on building plant scale equipment which later must be modified. The model does not replace the lab and pilot lab experiments necessarily, but may be used as a tool in order to reduce risk to capital expenditures. The

field of fluid dynamics, as applied to physical systems, in which more than one phase exist, is of particular interest to this research. Application of computational fluid dynamics of multi-phase to physical system has helped designers build safer and more economical equipment. In particular, computational fluid dynamics has contributed greatly to the development of a nuclear industry. In fact, much of the research in the two-phase flow was done explicitly to develop numerical codes to simulate loss of coolant situations and to simulate reactor cores for the nuclear industry. These numerical methods saved literally millions of dollars in experimental costs of designing safety systems by using the model to predict results that otherwise would have to be measured experimentally.

In this chapter a similar approach will be used as applied to a Vacuum Pan Sugar Crystallizer. The applied equations describing viscous two-phase flow with a free surface will be presented. These equations will be considered as adequately describing conditions promoting natural circulation in a Vacuum Pan Sugar Crystallizer. The numerical methods needed to solve the mathematical formulation of the problem will be developed and presented in another chapter. The development of the fluid dynamic equations describing two-phase flow under various assumptions has been done in the literature. Therefore, such development will not be done here, instead,

literature will be cited in order to indicate the available sources of information.

The one-dimensional homogeneous flow is the most basic of the fluid dynamic models of the two-phase flow phenomena. The basic assumption of this model is that the two-phase fluid can be presented as one fluid with proper averages applied to the physical properties. Wallis (1969) has a good applied presentation of this model. He continues his discussions of one-dimensional models with the two-phase stratified flow models. The stratified model considers each phase separately, but the equations are coupled by exchange functions that describe the exchange of mass, momentum, and energy across the interface. The development of multi-dimensional stratified and homogeneous models are done in detail in Ishii (1975). Ishii's approach is to develop the complete mathematical model of two-phase flow in as much detail as possible and then identify the areas where development of phenomenological models are needed to give closure to the set of equations. These phenomenological models describe the interchange of mass, energy, and momentum across the interfaces between phases. Each phase is considered a continuum. The results are a set of equations that based on the magnitude of certain dimensionless numbers can be simplified. Soo (1967) has written a book that is very comprehensive in the analysis

of applied multi-phase flow. Soo (1978) has also written an article in an attempt to bring out the distinguishing differences between continuum mechanics and multi-phase flow, Soo makes the point that only when the multi-phase mixture is considered as completely homogeneous can continuum mechanics be used to derive the models. Solbrig (1978) reviews the literature concerning the development of the applied two-phase flow equations and multi-phase flow equations. In addition, he also derives a set of equations. Because of the complexity of the multi-phase flow equations and their solution, the hope in developing a workable model in a limited amount of time and computer resources is bleak unless a great many assumptions can be made to simplify the complexities. Hopefully these assumptions can be justified.

The development of the mathematical model for the Vacuum Pan will be done in several parts as pertaining to several sections of the Pan. These sections are the Pan Proper, Downtake and Bottom, and Calandria (or tube section). The various sections of the Pan were discussed earlier in reference to Figure 1.0.0. The development of the model is done in this fashion to insure that the main characteristics of each section are modeled. Thus, when all the sections are combined, a model is formulated that describes the main characteristics of Pan operation without overkilling the simpler sections with complexity.

The formulation of the mathematical model for the free surface will be deferred to the chapter on the numerical model, since the differences in this section and the Pan Proper are only the results of the numerical solution technique.

Before stating any of the conservative equations of mass, energy, and momentum, some assumptions will be made and the conservative equations will reflect these assumptions from the outset. Further modifications and assumptions will be made if needed in subsequent discussions concerning sectionalization as mentioned above. These assumptions are listed below.

(1) Homogeneous flow of the mixture.
i.e., The solid and vapor phases are completely dispersed in the predominant liquid phase.

(2) All phases are moving with the same velocity.

(3) There is instantaneous thermal and mechanical equilibrium between all phases.

(4) Laminar flow exists.

(5) Newton's law of viscosity and Fourier's law of heat conduction apply.

(6) The viscosity terms reflect the incompressible nature of the liquid.
i.e., The substantial derivative of the density changes little spatially.

(7) The substantial derivative of the pressure is

negligible compared to the other terms in the energy equation.

(8) Viscous heating of the fluid is negligible.

(9) The heat of crystallization is negligible.

(10) No spatial variation of the concentration of sucrose, impurities, and crystals.

(11) The flow is axisymmetric with no circulatory motion about the vertical axis, therefore, two-dimensional with the coordinates being the radial and vertical directions.

(12) No nucleation of new crystals.

(13) The hydrostatic head assumption is applicable to reduce the vertical momentum equation to the density and pressure term.

3.1 OVERALL BALANCES

As indicated in assumption (10), no species continuity will be stated for the spatial variation of the concentration of sucrose, impurities, or crystals. The dynamics of these components will be described with Equations 3.1.1 thru 3.1.5, which are the lumped overall material balances for the whole Pan. The hold-up of vapor was assumed to be negligible and a overall material balance for the vapor was not written. The mass fractions of each component are calculated as according to Equations 3.1.6 thru 3.1.9. Since these overall mass balances were used instead of distributed balances, several assumptions will have to be made with regards to the calculation of mixture enthalpy and density, these assumptions will be discussed later.

sugar: $$\frac{dS}{dt} = F\ XSF - \frac{dC}{dt} \qquad 3.1.1$$

impurity: $$\frac{dIMP}{dt} = F\ XIMF \qquad 3.1.2$$

water: $$\frac{dW}{dt} = F\ XWF - ER \qquad 3.1.3$$

crystal: $$C = N_c\ \rho_c \frac{\pi}{6} L^3 \qquad 3.1.4$$

crystal size: $$\frac{d\bar{L}}{dt} = G \qquad 3.1.5$$

mass fractions:

$$XSP=S/TMASS \qquad 3.1.6$$

$$XIP=IMP/TMASS \qquad 3.1.7$$

$$XWP=W/TMASS \qquad 3.1.8$$

$$XCP=C/TMASS \qquad 3.1.9$$

The overall balances for the sugar, impurities, and crystal content were taken from a model developed by Wright (1974). However, Wright included dispersion of the CSD by an empirical equation. One of the objects of this research, is to show that the model for the fluid dynamics developed in this dissertation in combination with a distributed particle balance can calculate the dispersion of the CSD directly. Although, the particle balances discussed earlier were not programmed, the growth rate variations in the pan will be demonstrated in the results. As mentioned above, it is assumed that local variations in concentration of the sucrose and impurities are negligible, therefore, the cause of growth variations is assumed to result from the temperature differences in the Pan. These temperature differences have to be significant if natural convection is to be the mechanism to circulate the batch.

3.2 GENERAL HOMOGENEOUS MODEL

The homogeneous equations, as taken from Ishii (1975) page 229, after neglecting the effects of the interfaces on the momentum and energy equations, are presented below in vector form in Equations 3.2.1 thru 3.2.7.

continuity: $$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho U = 0 \qquad 3.2.1$$

momentum: $$\frac{\partial U}{\partial t} + \nabla \cdot \rho UU = -\nabla P + \nabla \cdot \boldsymbol{\tau} + F_B \qquad 3.2.2$$

energy: $$\frac{\partial \rho H}{\partial t} + \nabla \cdot \rho U H = K\nabla^2 T + \frac{DP}{Dt} + \phi_c \qquad 3.2.3$$

density: $$\rho = \Sigma \gamma_i \rho_i \qquad 3.2.4$$

velocity: $$U = \frac{\Sigma \gamma_i \rho_i U_i}{\rho} \qquad 3.2.5$$

enthalpy: $$H = \frac{\Sigma \gamma_i \rho_i H_i}{\rho} \qquad 3.2.6$$

stress tensor: $$\boldsymbol{\tau} = \mu(\nabla U + (\nabla U)^+) \qquad 3.2.7$$

Applying the following assumptions: (2), (4), (6), (7), (8), and (9), and transforming to the cylindrical coordinate system, Ishii's equations are reduced to Equations 3.2.8 thru 3.2.14. Equations 3.2.8 thru 3.2.14 are exactly the same equations that could be developed

under the assumptions above, if the single-phase equations from Bird, Stewart, and Lightfoot (1960) were simplified and the same mixing rules for the physical properties applied. These equations are offered as the general model for the Vacuum Pan Sugar Crystallizer under the assumptions applied. The boundary conditions for the system will be discussed later.

continuity: $$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial r\ \rho\ u}{\partial r} + \frac{\partial \rho w}{\partial z} = 0 \qquad 3.2.8$$

radial momentum: $$\frac{\partial \rho u}{\partial t} + \frac{1}{r}\frac{\partial r\ \rho\ u^2}{\partial r} \qquad 3.2.9$$
$$+ \frac{\partial \rho w u}{\partial z} = -\frac{\partial P}{\partial r} + \rho \nu \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2}\right)$$

vertical momentum: $$\frac{\partial \rho w}{\partial t} + \frac{1}{r}\frac{\partial r\ \rho\ u\ w}{\partial r} + \qquad 3.2.10$$
$$\frac{\partial \rho w^2}{\partial z} = -\frac{\partial P}{\partial z} + \rho \nu \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial w}{\partial r}\right) + \frac{\partial^2 w}{\partial z^2}\right) - g\rho$$

energy: $$\frac{\partial \rho H}{\partial t} + \frac{1}{r}\frac{\partial r\ \rho\ u\ H}{\partial r} \qquad 3.2.11$$
$$+ \frac{\partial \rho w H}{\partial z} = \rho \alpha \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right)$$

density: $$\rho = \Sigma\ \gamma_i\ \rho_i \qquad 3.2.12$$

velocity: $$U = U_i \qquad 3.2.13$$

enthalpy: $$H = \frac{\Sigma \gamma_i \rho_i H_i}{\rho} \qquad 3.2.14$$

3.3 SECTIONALIZATION

The general homogeneous equations presented above, along with other pertinent equations, fully describe the operation of the Vacuum Pan Sugar Crystallizer. But, application of these fully two-dimensional equations would lead to a very complex model. This complexity for all portions of the Pan is unwanted because the characteristics of each section differ. In the following sectionalization of the model, all equations can be simplified from the general homogeneous flow Equations 3.2.8 thru 3.2.11. However, the Pan Proper is the only section where the general equations can be most easily seen to apply. This is intentional because the Pan Proper is the most complex of the sections modeled.

a. Pan Proper

The Pan Proper makes up the largest volume of the Pan and exhibits the most spatial differences in the velocity and temperature profiles. Complex convection currents occur in this section resulting from the hot liquid rising from the Calandria and backmixing of the cooler liquid that has released its vapor at the surface. The modeling of the Pan would be completely inadequate if this section of the Vacuum Pan was treated as one lump.

Because of its distributed nature, this section will be modeled by applying the general model equations presented earlier. In addition to the assumptions inherent in Equations 3.2.8 thru 3.2.13, it is also assumed that the hydrostatic head assumption is adequate as a description of pressure profiles in the Pan Proper. Actually, this assumption neglects all the terms in the vertical momentum equation except the pressure and the body force terms, that is, the effects of inertia, convection of momentum, and the viscous forces are assumed negligible. The resulting equations are presented below in Equations 3.3.1 thru 3.3.4.

continuity: $$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial r \rho u}{\partial r} + \frac{\partial \rho w}{\partial z} = 0 \qquad 3.3.1$$

radial momentum: $$\frac{\partial \rho u}{\partial t} + \frac{1}{r}\frac{\partial r \rho u^2}{\partial r} + \frac{\partial \rho w u}{\partial r} = -\frac{\partial P}{\partial r} + \rho \nu \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial u}{\partial r}\right) - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2}\right) \qquad 3.3.2$$

vertical momentum: $$-\frac{\partial P}{\partial z} - \rho g = 0 \qquad 3.3.3$$

energy: $$\frac{\partial \rho H}{\partial t} + \frac{1}{r}\frac{\partial r \rho u H}{\partial r} + \frac{\partial \rho w H}{\partial z} = \rho \alpha \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right) \qquad 3.3.4$$

b. Calandria

The Calandria is basically a heating section and is generally made of a number of tubes into which massecuite flows vertically upward on the inside and is heated by condensing steam on the outside of the tubes. Since the radial distances of the Pan Proper are much larger than the radial distances of the tubes, each tube can be considered as one-dimensional.

Because each tube has a different radial position it may be subject to different conditions and thus, different conditions could exist in each tube. Considering each tube independently could cost a great deal of computer time and programming time, therefore, it was decided to use an average tube to represent all the tubes. The one-dimensional model for the tubes are presented below in Equations 3.3.5 thru 3.3.8. These equations are exactly the same as the model for a boiler tube given in Wallis (1969), but, the hydrostatic head assumption has been applied. However, the pressure drop due to friction has been retained because friction restricts flow in the tubes considerably. The laminar flow equation is used to calculate the pressure drop, if vapor is present the velocity of the liquid for the same mass flux will be used. The equation for the local friction pressure drop is given in Equation 3.3.8. The

equations below can also be derived directly from the general homogeneous flow equations presented earlier. This can be done by integrating the equations over the cross-sectional area of the tubes. Once the proper boundary conditions are applied, the resulting equations are identical to those below.

continuity: $$\frac{\partial \rho}{\partial t} + \frac{\partial \rho w}{\partial z} = 0 \qquad 3.3.5$$

vertical momentum: $$-\frac{\partial P}{\partial z} - \rho g - FR = 0 \qquad 3.3.6$$

energy: $$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho w H}{\partial z} = \qquad 3.3.7$$

$$\rho \alpha \frac{\partial^2 T}{\partial z^2} + UPOA(T - TSTEAM)$$

frictional pressure drop: $FR = 32 \mu w / D_t^2$ 3.3.8

c. Bottom

The Bottom and Downtake serve basically as a conduit to recirculate the massecuite back through the heating section. When modeling, several observations can be made. The conditions in this section are obviously non-boiling because the pressure is higher than the pressure in the Pan Proper that feeds this section. The dynamics of temperature changes are slow, since the profiles in the Pan Proper change only in response to the level of the Pan and the total solids fraction in the Pan which are slow dynamically. That is, assuming the two-phase boiling transients in the Pan Proper that occur on a small time scale have a negligible effect on the Pan Bottom and Downtake. In addition, most of the liquid that recirculates through the Downtake comes from the surface after it has boiled. Thus, the flux of liquid in the Bottom is of fairly constant temperature.

Since the conditions in the Bottom and Downtake are non-boiling and temperature changes are slow, it makes no sense to treat this area in a distributed fashion. Therefore, the Bottom and Downtake are treated as one lump for the energy and continuity equation. Because the effect of temperature on the density is small, the time derivative of the density in the continuity equation or mass balance for the Bottom and Downtake is neglected.

However, a problem occurs when writing the unsteady lumped momentum balance as presented in Bird, Stewart, and Lightfoot (1960), and presented in Equation 3.3.9. The formulation of the equation is made in reference to Figure 3.3.1.

$$\frac{\partial P}{\partial t} = (P + \rho w^2)_1 A_1 - (P + \rho w^2)_5 A_5 - FR_{1-5} + F_{B\ 1-2} \qquad 3.3.9$$

The problem results from the fact that there is no specific cross-sectional area to base the momentum in the radial Pan Bottom. Splitting the Equation 3.3.9 into two lumps, Equations 3.3.10 for the Downtake and Equation 3.3.11 for the Bottom, isolates the problem in determining the lumped inertial term to Equation 3.3.11.

$$\frac{\partial P}{\partial t}\ 1\text{-}2 = (P_1 - P_2)A_1 - FR_{1-2} + \rho A_1\ TUBEH\ g \qquad 3.3.10$$

$$\frac{\partial P}{\partial t} 2\text{-}5 = (P + \rho w^2)_2 A_2 - (P + \rho w^2)_5 A_5 - FR_{2-5} \qquad 3.3.11$$

The inertial term in Equation 3.3.11 cannot be determined without knowing the velocity profiles in the Pan Bottom. This means a lumped analysis will not allow the inertial term to be evaluated. If the lumped momentum analysis is to be used for the Bottom, the inertial term in Equation 3.3.11 will have to neglected, thus, a steady

state assumed. In order to maintain the dynamics of the problem and avoid the problem with Equation 3.3.11 in determining the inertial term, the cross-sectional area between the Downtake and the Calandria is taken as a basis for a one-dimensional momentum balance. Referring to Figure 3.3.1 will pin point the area under discussion. Equation 3.3.12 is the one-dimensional momentum balance for this section of the Pan, it can be obtained from Equation 3.2.9 by neglecting all the derivatives in the vertical direction. Equation 3.3.12 can be integrated over this area by applying the continuity equation for the cross-section to obtain the momentum at each point. Equation 3.3.18 is the resulting equation, the steps for its derivation are outlined in Equations 3.3.13 thru 3.3.17.

In the derivation of Equation 3.3.18, each of the terms in Equation 3.3.12 are integrated over the volume between point (3) and (4) i.e., V_{34}. The dynamic term, Equation 3.3.14, is integrated by applying Leibnitz's Rule (Bird, Stewart, and Lightfoot (1960)). The bar over the radial velocity indicates that it is the volume averaged radial velocity, for convenience this will be taken as being evaluated at the average radial position between points (3) and (4). Likewise, the pressure term is evaluated similarly. The gradient of pressure is then approximated assuming pressure to be a linear function of radial position. The viscous terms drop out directly by

applying Equation 3.3.13.

$$\frac{\partial u}{\partial t} = - u \frac{\partial u}{\partial r} - \frac{1}{\rho} \frac{\partial P}{\partial r} + \nu \left(\frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial u}{\partial r}\right) - \frac{u}{r^2}\right) \qquad 3.3.12$$

$$r\, u = c_1 \qquad 3.3.13$$

$$\int_{V_{3-4}} \frac{\partial u}{\partial t}\, dV = \frac{\partial \bar{u}}{\partial t}\, V_{3-4} \qquad 3.3.14$$

$$-\int_{V_{3-4}} u \frac{\partial u}{\partial r}\, dV = - c_1^2 \left(\frac{1}{r}\right) \Bigg]_{r_3}^{r_4} 2\pi \text{ BOTTH} \qquad 3.3.15$$

$$- \frac{1}{\rho} \int_{V_{3-4}} \frac{\partial P}{\partial r}\, dV = - \frac{\overline{\Delta P}}{\Delta r}\, V_{3-4} \qquad 3.3.16$$

$$\frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{u}{r}\right) - \frac{u}{r^2} = 0 \qquad 3.3.17$$

$$\frac{\Delta \bar{u}}{\Delta t} = -\frac{1}{\rho} \frac{\overline{\Delta P}}{\Delta r} - 2 c_1^2 \left(\Delta \frac{1}{r}\right) / (\Delta r^2) \qquad 3.3.18$$

The use of Equation 3.3.18 requires an assumption concerning the pressure profile, refering to Figure 3.3.1, from point (2) to point (3) and from point (4) to point (5). Since the flow is slow and the pressure drop across the area between the Downtake and the Calandria is, by pan design, small, it is assumed that the pressure at point (2) is equal to the pressure at point (3) and the pressure at point (4) is equal to the pressure at

point (5).

In summary, the equations modeling the Downtake and Bottom are presented in Equations 3.3.19 thru 3.3.22. Equation 3.3.19 is the lumped energy equation. Equation 3.3.20 is the continuity relation or the mass balance for the Downtake and Bottom. The momentum and equations are split into Equation 3.3.21 for the Downtake and Equation 3.3.22 for the Bottom. The continuity relation for the one-dimensional section in which Equation 3.3.22 is based on is Equation 3.3.13. Notice that Equations 3.3.19 and 3.3.20 reflect the input of mass and energy by the feed. The momentum of the feed is neglected.

energy: $$\rho V \frac{dH}{dt} = (- \rho w)_1 H_1 \quad 3.3.19$$

$$- (\rho w)_5 H_5 + F HF$$

continuity: $$(\rho w)_5 A_5 = (\rho w)_1 A_1 \quad 3.3.20$$

$$+ F$$

vertical downtake: $$P_2 = P_1 + FR_{1-2} \quad 3.3.21$$

$$+ \rho \text{ TUBEH } g \qquad FR_{1-2} = \frac{8 \mu w \cdot TUBEH}{R_{dwn}^2}$$

radial momentum bottom: $$\frac{d\bar{u}}{dt} = - \frac{1}{\rho} \frac{(P_5 - P_2)}{(r_4 - r_3)} \quad 3.3.22$$

$$- 2 (\bar{r}\ \bar{u})^2 (\Delta \tfrac{1}{r}) / (\Delta r^2)$$

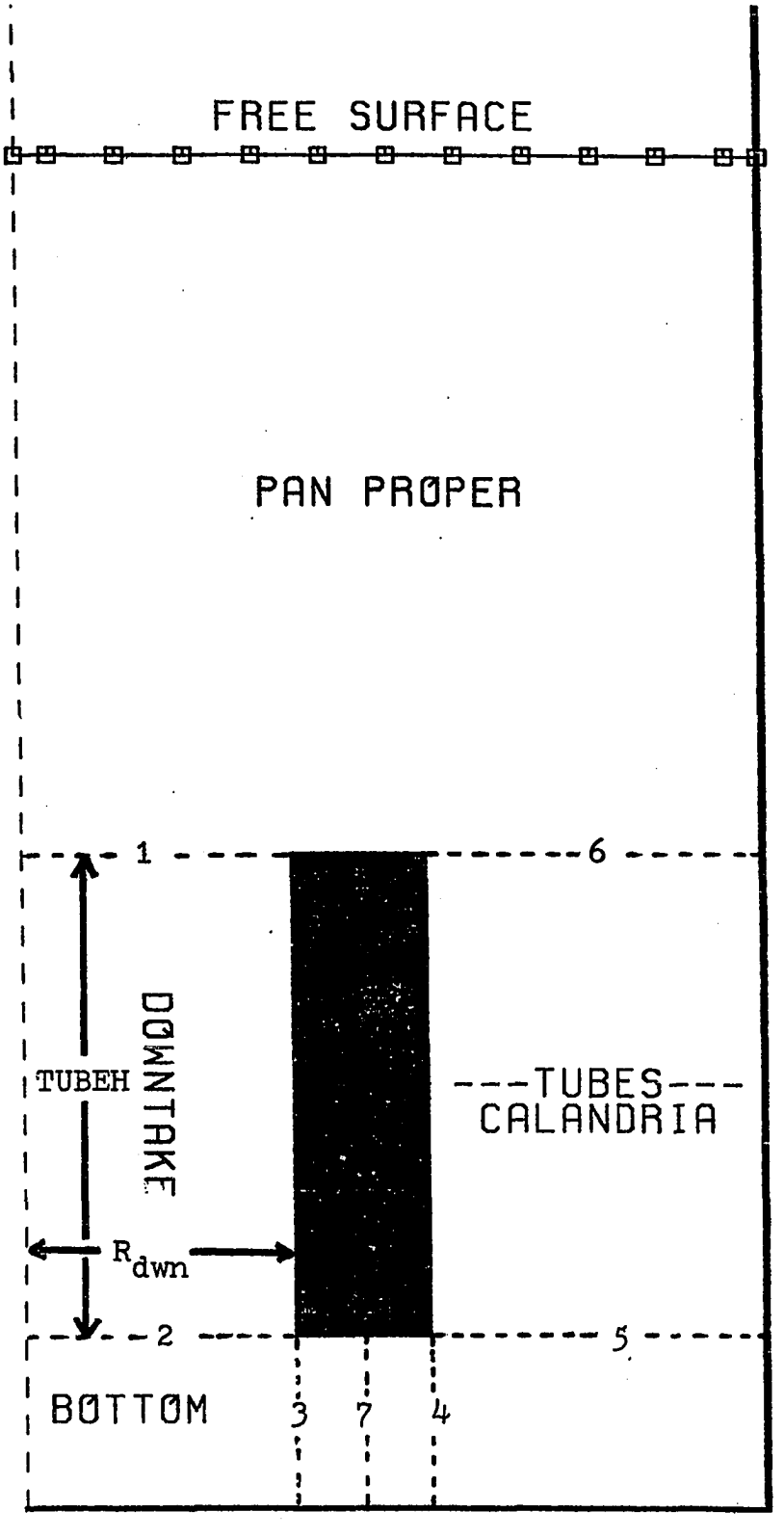


FIGURE 3.3.1 SECTIONALIZED VACUUM PAN

3.4 PERTINENT EQUATIONS

In order to give closure to the set of equations presented earlier and distinguish the model for application to an Industrial Vacuum Pan Sugar Crystallizer, certain pertinent equations are needed. These equations include a mathematical definition of the equations of state, thermodynamic state, kinetics, equilibrium conditions, and heat transfer relationships. These relationships will be supplied in the following discussions.

a. Equations Of State Three-Phase System

The proper average density for the homogeneous model has been given in Equation 3.2.4. The average density is the volume average of the component densities. Equation 3.2.4, however, which is implicit in the average density, for computational reasons is not in a good form. Assuming there is no volume change due to mixing, the mixture volume is the sum of the component volumes. Equation 3.4.1 states the alternate form of Equation 3.2.4, which is in a better computational form. Multiplying Equation 3.4.1 through by the mixture density defines the volume fraction of each component as shown in Equation 3.4.2.

$$\frac{1}{\rho} = \Sigma \frac{x_i}{\rho_i} \qquad 3.4.1$$

$$\gamma_i = \frac{x_i \rho}{\rho_i} \qquad 3.4.2$$

During the operation of the Pan there is the possibility of the three phases. Those phases are an aqueous solution of sugar, sugar crystals, and water vapor. It is assumed that the water vapor density can be adequately explained for pressure and temperature changes relative to a reference density as suggested by the Ideal Gas Law. But since pressure in the Pan may more than double from top to bottom of the Pan, while temperature effects are not so drastic, the equation of state for the vapor will be presented by Equation 3.4.3. This equation corrects only for pressure changes on the reference density. For computation convenience the reference density is evaluated at temperature and pressure of the vapor space.

$$\rho V = \rho VR\left(\frac{P}{PR}\right) \qquad 3.4.3$$

The sugar crystal density given in Honig (1963) as 1.588 g/ml.

An extensive equation of state for sugar solutions was not found in the literature. Because of the limited range of temperature and sucrose concentration of

interest, a Taylor series expansion of the effects of these variables will be adequate. The liquid is assumed to be incompressible. Equation 3.4.4 is the Taylor series expansion truncated after the first term. Equation 3.4.5, the dimensionless form of Equation 3.4.4, is found by dividing the equation through by the reference density. The two parameters in the equations are then identified as the coefficient of thermal expansion and the coefficient of concentration.

$$\rho L = \rho LR + \frac{\partial \rho L}{\partial T}\Delta T + \frac{\partial \rho L}{\partial S}\Delta S \qquad 3.4.4$$

$$\rho L = 1 + \beta \Delta T + \beta_c \Delta S \qquad 3.4.5$$

Both of these coefficients are functions of the temperature and concentration, but, only change a percent or so for typical changes about the base point that occur in the Pan during its operation. The reference temperature and concentration are variables that can be changed to reflect the conditions in the Pan for a particular simulation. Table 3.4.1 and 3.4.2 show functionality of the parameters with temperature and concentration. However, the effect of temperature on the coefficient of concentration was omitted, because its effect was insignificant compared to the effect of concentration. As can be seen in the Tables, the

insensitivity of the parameters to changes in temperature and concentration of sucrose is apparent. Therefore, the truncated Taylor series should serve well to describe the density of the sucrose solution over the limited conditions of the evaporator.

For computational convenience also, the water and sucrose density plus the crystal density will be combined into one density and considered as one phase. The reasons for this will be made clear when the enthalpy of the three-phase system is discussed. Equation 3.4.6 reflects this computational convenience.

$$\frac{1}{\rho_{LS}} = \frac{1-XCP}{\rho_L} + \frac{XCP}{\rho_C} \qquad 3.4.6$$

TABLE 3.4.1: Coefficient of Concentration

BRIX	βC (1/BRIX)
.7	0.4611
.75	0.4635
.80	0.4655

TABLE 3.4.2: Coefficient of Thermal Expansion

	$\beta \times 10^4 (1/(F))$		
	TEMPERATURE (F)		
BRIX	131	149	185
.60	2.50	2.40	2.90
.75	2.46	2.62	2.86

b. Enthalpy Of Three-Phase System

The proper enthalpy per unit mass for the homogeneous model was presented earlier in Equation 3.2.6. However, like the density it is not in a good computational form. By direct substitution of the definition of the volume fraction, Equation 3.4.2, Equation 3.4.7 is derived that has computational advantages.

$$H = \Sigma x_i H_i \qquad 3.4.7$$

Although the system is three-phase, the enthalpy will be treated as the density was earlier. That is, the liquid and the crystals will be treated as one-phase but distinquished from the vapor phase as shown in Equation 3.4.8.

$$H = (1-XV)\ HL + XV\ HV \qquad 3.4.8$$

The enthalpy of the liquid and crystal mixture will be calculated via the heat capacity and temperature of the mixture. The heat capacity as represented by Equation 3.4.9 is taken from Hugot (1972). Equation 3.4.10 is the mathematical expression for the enthalpy of the liquid crystal mixture. The enthalpy of the vapor is by Equation 3.4.11.

$$CP = 1.0 - XSP(0.6 + XCP/0.6) \qquad 3.4.9$$

$$HL = CP(T - TR) \qquad 3.4.10$$

$$HV = 1075.8 + 0.43465(T - 32) + 1.4877x10^{-5}(T-32)^2 - 7.048x10^{-7}(T-32)^3 + SH \qquad 3.4.11$$

$$^{*}SH = 3.756599\ P\ BPE + 0.44973521\ BPE - 6.9478x10^{-5} BPE\ P^2 - 6.959x10^{-6} P\ BPE^2$$

Notice the correlation for the vapor enthalpy has a correction for the amount of superheat. This is needed, assuming that the vapor will be in thermal equilibrium with the sugar solution which is boiling at an elevated temperature due to the presence of the sucrose and impurities.

The equilibrium relationship to distinguish when the vapor phase may be present is the boiling point of the sucrose, impurity, and water solution. Since the enthalpy of the vapor is greater than the liquid and crystal mixture, the vapor enthalpy will always contribute to an excess enthalpy. Therefore, once the boiling point is reached, the temperature of the mixture is given by Equation 3.4.12 and the excess enthalpy is given to the vapor. The calculation of the mass fraction is, thus, explicit via Equation 3.4.13.

* NOTE: Pressure expressed in psia.

$$T = f(P) + BPE \qquad 3.4.12$$

$$XV = \frac{(H - HL)}{(HV - HL)} \qquad 3.4.13$$

The equilibrium boiling point of the sucrose, impurity, and water solution is given by the saturation temperature of the water at the same pressure, plus, a boiling point elevation due to the presence of the sucrose and impurities in the water. These relationships are given below in Equations 3.4.14 thru 3.4.16. The boiling point elevation of the solution is the superheat needed to calculate the vapor enthalpy in Equation 3.4.11.

boiling point elevation: 3.4.14

$$BPE = 2.2\frac{(XIP+XSP)}{XWP} + 1.1\frac{XIP}{(XSP+XIP)}$$

temperature of water: 3.4.15

$$^{*}TW = \frac{3061.596}{(6.306699 - \log P)} - 383.7148$$

boiling point of solution: 3.4.16

$$T = TW + BPE$$

* note: Pressure expressed in psia.

As mentioned earlier, no specie calculation will be done for the sucrose, crystal, or impurities. Strictly speaking, the concentration of these components will change locally as the local vaporization occurs. Therefore, this formulation is restricted to small mass

fractions of vapor, vaporizing at any one time. However, this should not be viewed as a restriction, given the homogeneous flow assumption is valid, because small mass fractions of vapor cause large changes in the mixture density. In fact, a mass fraction of only 10^{-4} can cut the mixture density in half and at the same time only have a minute effect on the calculation of the heat capacity of the crystal and liquid mixture or the boiling point. Because of the large effect of the presence of vapor on the mixture density, it is hard to imagine mass fraction much larger than 10^{-4} in a natural convecting environment.

c. Viscosity Liquid and Solid Mixture

The viscosity of the mixture of sugar solution and the sugar crystals is the main reason for the poor recirculation through the tubes and low heat transfer coefficients observed in the Vacuum Pan. In addition, the viscosity is an integral part of some of the approaches taken in literature for the analysis of the kinetics of crystal growth. Therefore, the importance of a good equation for the dependence of the viscosity on temperature, concentration of the sugar solution, and the presence of crystals is obvious. A correlation for the liquid viscosity was taken from work by Evans (1970), but was found not to reproduce the viscosity data in Honig (1963) very well. Since the range of concentration and temperature encountered in the Pan are small, it was decided to take the form of the equation presented in the article by Evans and use it to correlate the data in Honig. An optimization program was used to select the parameters that minimize the sum of the squares differences between the experimental data and the value predicted by the equation. The statistics concerning that optimization are presented in Table 3.4.3. The correlation coefficient, as defined in Miller (1965), of the experimental data against the proposed equation is 0.97. Statistical weights were used to aid in

finding a better correlation. These weights were assumed to be proportional to the magnitude of the viscosity to reflect the percentage error in the viscometer measurement. The data points used to develop the correlation are given in Table 3.4.4. This is only a fraction of the data presented in Honig, the data that were more representative of the conditions in the Pan were used to find the parameters. The reason for using the restricted sample is because it was felt that the functionality of the viscosity is really more complicated, and using all the data available for the optimization would not allow the equation to predict the viscosity accurately in the range of interest. It also should be mentioned that data in Honig does not include supersaturated conditions, therefore, the equation will be used to extrapolate the data. Equation 3.4.17 is the equation for liquid viscosity.

$$\mu L = EXP(10195.02/(T+460.) + 18.86(XSP+XIP)/(1-XCP) - 26.523)6.72x10^{-4} \quad 3.4.17$$

The presence of solid crystals has an effect on the apparent viscosity of the mixture. This effect will be corrected by a multiplying factor. This multiplying factor is given by Equation 3.4.18, taken from work by Awang (1976).

$$\frac{\mu}{\mu L} = \text{EXP}(8.959873 \text{ VCL } L^{0.15}) \qquad 3.4.18$$

Equation 3.4.17 will be used to calculate the liquid viscosity when needed in the program. Equation 3.4.18 will correct the liquid viscosity for the presences of crystals for pressure drop calculations or when kinematic viscosity is needed.

TABLE 3.4.3: Viscosity Correlation Statistics

TOTAL SUM SQ.	RESIDUAL SUM SQ.	CORREL. COEFF.
9379	26	0.97

NO. PARAMETERS=3 NO. POINTS=18

TABLE 3.4.4: Viscosity Data

	VISCOSITY(CP)		
	TEMPERATURE(F)		
BRIX	140	158	176
.70	39.1	25.1	16.9
.71	46.7	29.5	19.6
.72	56.3	35.0	22.9
.73	68.6	41.8	27.0
.74	84.4	50.5	32.1
.75	105	61.6	38.4

d. Solubility And Kinetics Of Sucrose In Water

There are several different sources of the kinetics of sucrose crystals. Smythe (1971) has obtained data for sucrose crystallization in pure solutions as well as solutions with various impurities and additives, as well as, reviewing the literature concerning research in sucrose growth kinetics. His data were taken under conditions that eliminate the effects of mass transfer of the sucrose to the crystal surface. He did this in order to study the kinetics of the surface integration step. However, in an operating Pan the rate of growth of a crystal is limited by mass transfer as well as the surface kinetics. This was shown to be true by Buchler (1980), who took experimental growth rate with crystals in an environment similar to that found in an operating Pan. Hartel (1979) has obtained experimental data for pure sucrose solutions from a continuous well stirred tank. His analysis of the data from his experiments were based on the concepts presented in Chapter 2. The correlation for the growth rate of sucrose crystals that will be used in the model was obtained from an article by Wright (1974). The model is correlated from industrial data and includes the effects of impurities and temperature. The equation includes the mass transfer step and the surface integration step because the total

difference in concentration or oversaturation is used. The mass average linear growth rate of an equivalent spherical crystal was used for the correlation to avoid the problem of the crystal shape. The reason for using Wright's model was its applicability to industrial Pans and its simplicity. The model is presented below in Equations 3.4.19 thru 3.4.22.

$$G = \frac{dL}{dt} = \begin{cases} k_G\ OS & OS>0 \\ 5k_G\ OS & OS<0 \end{cases} \qquad 3.4.19$$

$$k_G = k_G^0 EXP\left(-\frac{EACT}{2.303\ R_g}\left(\frac{1}{(T+460)} - \frac{1}{599.7}\right)\right) \qquad 3.4.20$$

$$EACT = 11.0 - 0.011111(\ T - 140\ ) + 8.0\ XIP/XWP \qquad 3.4.21$$

$$k_G^0 = 2.43x10^{-2} EXP(\ 1.75\ XIP/XWP\ ) \qquad 3.4.22$$

$$R_g = 1.104 \times 10^{-3}$$

As suggested by the model above, crystals only grow when exposed to a supersaturated environment of sucrose. Supersaturation is a measure of the excess amount of the sucrose above that when the solution is saturated. Therefore, the saturation point of the sucrose in water is of vital importance in order to determine when, and by what rate a crystal will grow. The saturation condition for pure

sucrose and water system is given by Equation 3.4.23, as taken from Wright's model.

$$SAT = 63.8188 - 5.1082\times10^{-3}T + 7.836\times10^{-4}T^2 - 1.5492\times10^{-6}T^3 \qquad 3.4.23$$

The calculation of supersaturation must be consistent with the model for the growth rate of the crystal. Since Wright's model for the growth rate is used as presented above, the supersaturation relationships from Wright's article will also be used. These relationships are presented below in Equation 3.4.24 and 3.4.25.

$$SS = \frac{(100-SAT)}{SAT}\left(\frac{XSP}{XWP}\right)\left(\frac{1}{1-0.88XIP/XWP}\right) \qquad 3.4.24$$

$$OS = SS - 1 \qquad 3.4.25$$

e. Heat Transfer Coefficients

Studies of heat transfer in Vacuum Pans are much lacking in the literature. No research has been done to quantify the mechanism of heat transfer in the tubes of the Vacuum Pan. The reason for this is partly because there has been no real need for accurate correlations for basic design. Also, it is partly because of the complexity of the problem. The heat transfer coefficients presented in Honig (1963), Hugot (1972), and Meade (1963), are based on steam consumption and the temperature difference between the steam and the temperature of the saturated liquid at the pressure of the pan vapor space. The absence of correlations for heat transfer coefficients, based on the local conditions in the tubes, will not prevent the development of the model or its subsequent use. But, without such local heat transfer coefficients, the effect of the pan level, steam temperature, and other operating conditions on heat transfer in tubes cannot be simulated properly. Since the heat load is the forcing function causing the flow, it seems important that the mechanism of heat flow be understood. Therefore, the need for research in this area is apparent.

While heat transfer in Vacuum Pans has not been studied extensively, evaporators have. Correlations have been given in a number of sources, Honig (1963),

Zagrodzki (1977), Saranin (1954), and Badger (1939). Unfortunately, these correlations do not extend into the range of operation of the Vacuum Pan. However, studying these correlations may help in understanding the effects of the physical properties of the mixture and the effect of operating conditions on heat transfer in the Pan.

For the purposes of the development and demonstration of the numerical model, typical values of the evaporation coefficients will be used to calculate the heat input to the Pan. The evaporation coefficient is defined as the rate of steam consumed per unit heat transfer area. Typical values of the evaporation coefficient for various purity massecuites, as taken from Hugot (1963), are summarized in Table 3.4.5.

TABLE 3.4.5: Evaporation Coefficient

	ECOEFF (LBS/FT^2/HR)	
	MAX	MIN
A MASSECUITE	14.6	6.6
B MASSECUITE	9.4	2.2
C MASSECUITE	7.5	0.34

3.5 NON-DIMENSIONALIZATION AND BOUNDARY CONDITIONS

In general, when solving a set of differential equations with numerical methods, the numerical solution is aided by putting the equations in dimensionless form. Picking the proper dimensional groups aids in reducing truncation errors because the dimensionless variable is scaled by the dimensional group. In some cases numerical solution speed is increased by picking dimensional groups involved in functional evaluations in the numerical code. In all cases, working with dimensionless equations adds a degree of flexibility in using the numerical coding of the equations, because the code no longer depends on units and at the same time, errors associated with dimensional inconsistency are reduced.

For the most part, the dimensional groups used here are adopted from Waldrop (1972) and Pitts (1976). However, dimensional groups were needed resulting from the variables associated with the energy equations for the Pan Proper and the Calandria. The non-dimensional forms of the variables are presented below in Table 3.5.1, as indicated by the prime mark. Applying these dimensional groups to the previously defined model equations, a non-dimensional set of equations are formulated. The non-dimensional equations appear the same as the dimensional equations and therefore, will not be repeated again.

Equation 3.1.1 thru 3.1.5 are not non-dimensionalized. These equations interact with the other equations only through the mass fractions which are already non-dimensional.

To complete the development of the model, the boundary conditions are presented in Table 3.5.2, Equations 3.5.15 thru 3.5.58. The table includes spatial as well as temporal boundary conditions. These initial conditions in combination with the spatial boundary conditions are necessary conditions that must be specified if a solution is to be attempted. The spatial boundary conditions, in some cases, are based on physical reasoning and in other cases, to insure the conservation of mass, energy, and momentum between sections. A discussion of the spatial conditions are given below.

For the Pan Proper, at the surface, the conditions of no normal or tangential viscous stresses are imposed. The exchange of mass, momentum, and energy between all modeled sections including the vapor space, which was not modeled, is done only through the convective terms. The only exception to this rule is at the top of the Calandria, at this point, thermal conduction is allowed because substantial temperature gradients can exist. At the center for the Pan Proper, the radial velocity is zero and symmetry is insured by making the enthalpy, vertical velocity, and pressure derivatives in the radial

TABLE 3.5.1: Non-Dimensional Variables

$$T' = T\beta/CPW \qquad 3.5.1$$

$$H' = H\beta/CPW \qquad 3.5.2$$

$$\mu' = \mu \,/\, R/hmax/\sqrt{hmax\ g} \qquad 3.5.3$$

$$\kappa' = \kappa/CPW/\ R/hmax/\sqrt{hmax\ g} \qquad 3.5.4$$

$$\nu' = \nu/hmax/\sqrt{hmax\ g} \qquad 3.5.5$$

$$\alpha' = \alpha/hmax/\sqrt{hmax\ g} \qquad 3.5.6$$

$$r' = r/hmax \qquad 3.5.7$$

$$z' = z/hmax \qquad 3.5.8$$

$$U' = U/\sqrt{hmax\ g} \qquad 3.5.9$$

$$t' = t/\sqrt{hmax/g} \qquad 3.5.10$$

$$\rho' = \rho/\rho R \qquad 3.5.11$$

$$P' = P/hmax/\rho R/h \qquad 3.5.12$$

$$CP' = CP/CPW \qquad 3.5.13$$

$$h' = h/hmax \qquad 3.5.14$$

$$UU' = UU/CPW/\rho R/\ hmax/g \qquad 3.5.15$$

direction equal to zero. At the walls, slip conditions are applied because for the most part, the numerical solutions will be done with large grid spacing, thus, the wall should have little influence on the point on the order of a foot away. The same reasoning was applied for the area across the bottom of the Pan Proper. In addition, the temperature gradient normal to the wall is taken as zero to indicate no conduction of heat through the wall. The velocities at the wall are zero. The pressure gradient in the radial direction normal to the wall is taken as zero. Refer to Figure 3.3.1 to clarify the notation concerning the boundary conditions for the Downtake and Calandria.

The most interesting of the boundary conditions are Equations 3.5.18 thru 3.5.20 involving the release of mass, momentum, and energy at the surface. These equations employ a functional relationship between the relative velocity of the vapor to the liquid and the volume fraction vapor at the surface. The function is taken from the literature and is typically used in the drift flux models as described in Wallis (1969) and Ishii (1975). The form of the function used in this research, describing the velocity of vapor relative to the surface, is shown in Equation 3.5.51

$$w_v - w_s = W_v^* (1-\gamma)^n \qquad 3.5.51$$

The parameters in Equation 3.5.51, W_v^* and n, are a function of the evaporation rate, the physical properties of the fluid and the vapor bubble size. Experimental work is needed to establish the magnitude of these parameters for the conditions in the Pan. Therefore, for computational convenience, n is assumed to be zero and W_v^* is given sufficient magnitude such that the maximum evaporation rate can exceed the heat input.

TABLE 3.5.2: BOUNDARY CONDITIONS

SURFACE

$$\frac{\partial T}{\partial z} = 0 \quad \frac{\partial w}{\partial z} = 0 \quad \frac{\partial u}{\partial z} = 0 \qquad 3.5.15\text{-}3.5.17$$

$$\rho V(w_v - w_s) = \rho V f(\gamma) \qquad 3.5.18$$

$$\rho V(w_v - w_s)HV = \rho V HV f(\gamma) \qquad 3.5.19$$

$$\rho V w_v = (f(\gamma) + w_s)\rho V \qquad 3.5.20$$

$$P = P_s \qquad 3.5.21$$

WALLS

$$\frac{\partial H}{\partial r} = 0 \quad \frac{\partial P}{\partial r} = 0 \quad \frac{\partial T}{\partial r} = 0 \qquad 3.5.22\text{-}3.5.24$$

$$\frac{\partial u}{\partial r} = 0 \quad \frac{\partial w}{\partial r} = 0 \quad u = 0 \qquad 3.5.25\text{-}3.5.27$$

CENTER LINE

$$u = 0 \quad \frac{\partial P}{\partial r} = 0 \quad \frac{\partial H}{\partial r} = 0 \qquad 3.5.28\text{-}3.5.30$$

$$\frac{\partial T}{\partial r} = 0 \quad \frac{\partial u}{\partial r} = 0 \quad \frac{\partial w}{\partial r} = 0 \qquad 3.5.31\text{-}3.5.33$$

DOWNTAKE - PAN PROPER

$$\frac{\partial T}{\partial z} = 0 \quad \frac{\partial w}{\partial z} = 0 \quad \frac{\partial u}{\partial z} = 0 \qquad 3.5.34\text{-}3.5.36$$

$$u = 0 \quad w = w_1 \quad \rho = \rho_1 \qquad 3.5.37\text{-}3.5.39$$

$$H_1 = \int H dA_1 \qquad 3.5.40$$

CALANDRIA - BOTTOM

$$\frac{\partial T}{\partial z} = 0 \quad \frac{\partial w}{\partial z} = 0 \quad \rho = \rho_5 \qquad 3.5.41\text{-}3.5.43$$

$$\rho w A = \rho_5 w_5 A_5 \quad H = H_5 \qquad 3.5.44\text{-}3.5.45$$

CALANDRIA - PAN PROPER

$$\frac{\partial w}{\partial z} = 0 \quad \frac{\partial u}{\partial z} = 0 \quad u = 0 \qquad 3.5.46\text{-}3.5.48$$

$$\rho w A = \rho_6 w_6 A_6 \quad H = H_6 \quad T = T_6 \qquad 3.5.49\text{-}3.5.51$$

INITIAL CONDITIONS

$$I = I_o \quad S = S_o \quad C = C_o \quad W = W_o \qquad 3.5.52\text{-}3.5.55$$

$$H = H_o \quad U = U_o \quad P = P_o \qquad 3.5.56\text{-}3.5.58$$

3.6 DISCUSSION OF THE ASSUMPTIONS

As presented earlier, many assumptions were made in the derivation of the mathematical model. These assumptions must be kept in mind when applying the model. The fluid dynamics of an operating Vacuum Pan are very complicated, the liquid is very viscous and contains solid particles and may be boiling vigorously. The hope of developing a numerical model that captures the minute details of the fluid dynamics of the Crystallizer, and be practical in terms of use of limited computer facilities is unrealistic. This problem prompted the assumptions used in the derivation of the model.

One of the fundamental assumptions made is the assumption of homogeneous flow. The homogeneous flow assumption represents the mixture of solids, liquid, and vapor as a quasi-fluid with physical properties that are mass averages of the species physical properties. This basically limits the calculation validity to a low volume fraction of vapor because when a large fraction of vapor exists, the vapor phase tends to separate. The effect of high volume fractions of crystals is not so critical because the high liquid viscosity restricts the tendency of the crystals to separate. Because the vapor phase tends to separate when the volume fraction of the vapor is large, the homogeneous model over estimates the mass average velocities

caused by buoyancy effects and the fluid drag caused by velocity gradients. This results because the vapor moves considerably faster than the liquid and solid phases but contributes greatly towards reducing mixture density. Further assumptions concerning the numerical flash calculation are valid only for low mass fractions of vapor (10^{-3}), because the solids and liquid phases are assumed to be one-phase in this calculation and neither the solid phase mass fraction nor the concentration of soluble sugar in solution are changed to find the real equilibrium position. However, the flash calculation is not a real limitation because the homogeneous assumption is much more limiting, besides, it is difficult for large vapor fractions to exist in the Pan Proper because vigorous mixing occurs when the vapor phase is present, and in most circumstances the heat input is too low to cause much flashing in the tubes.

The model also assumes that there is equilibrium between the phases and it occurs instantaneously. These assumptions are valid for all but very fast and highly accelerating flow and when the phases become separated. Although, Batterham (1975) indicates that there is evidence of measurable superheat in the Pan, its effect on the flow is small because the superheat is not large. Significant non-equilibrium between phases is also assumed to be small because the flow is slow and the heating rate

is low.

The model also neglects the heat loss to the environment by conduction through the walls of the Vacuum Pan, and the heat of crystallization. These effects are estimated to be about 5% of the total heat loads. However, these effects can be added easily enough if desired.

Another most important assumption of the model is the hydrostatic head assumption for the pressure profile. This assumption reduces the vertical momentum equation to only the density term and the pressure term. This assumption is common in the literature for modeling bays and estuaries as discussed by Pitts (1976). While it is true that these two terms are the dominant terms in the equation, the derivative of the vertical momentum equation with respect to the radial direction is the proper way to analyze the effect of these terms on the pressure profile. It becomes evident in this light that the other terms may be important depending on the flow, especially the convective terms. The application of the hydrostatic head assumption to fluid dynamics of the Vacuum Pan will have to be evaluated once the numerical model of the Pan has been developed.

CHAPTER 4

COMPUTATIONAL METHODS

In Chapter 3, a mathematical model of a Vacuum Pan Sugar Crystallizer was developed. The model is based on the fundamentals of the physics of fluid motion and the phenomena of two-phase flow. In this chapter, the discrete analogs of the governing equations will be derived. These discrete equations will form the base for the numerical solution of the governing equations. The development of the numerical methods as taken from the literature pertaining to this research will be overviewed to contrast the development here. These references will supply a wealth of information concerning numerical methods in computational fluid mechanics. Although the computer code will be attached in the appendix, the calculation sequence will be presented in enough detail to insure understanding.

The development of the numerical codes for multi-phase flow has been somewhat predicated upon the development of the codes for single-phase compressible and incompressible flow. This of course, results from the fact that, historically, the codes for single-phase flows were developed and tested first and their success dictates further application. Since typically, free surface flow multi-phase flow, and compressible flow calculations have

been done by directly solving the primitive equations, i.e., the equations of motion without transforming the variables, the discussion and references will be directed towards the solution of the primitive equations. The development of discrete analog equations and solution methods for the single-phase flow primitive equations are extensive in the literature. Several good references for these finite differencing and solution methods are Roache (1976), MacCormack (1978), Warming (1978), and Patankar (1980).

A particularly complex problem addressed in the context of incompressible fluid flow is the moving boundary or free surface problem. Such problems are exemplified by the presence of an interface. For the purposes here, the free surface problem will be typified by a cavity of a fluid, such as liquid in a partially filled tank or a large body of water, where in both cases the surface changes position in reaction to the forces which act upon it. The Los Alamos group developed the Marker Cell Method (MAC) to solve this class of problems. It is by far the most popular method to solve incompressible flow free surface problems. The method and its development are discussed in Roache (1976). The MAC method is quite general and capable of solving a wide variety of problems such as, waves crashing on the beach, dams breaking, and solid objects rising and falling in

liquids. Although a fixed grid system is used, the interface is simulated by adding or substracting surface cells as the fluid flow suggests.

The MAC method uses the Poisson Equation to solve for the pressures and employs marker particles, which flow with fluid but do not affect the fluid dynamics, to locate the surface cells. The difficulty with the MAC method and its derivatives is that the solution is very complex and time consuming. This results because the solution of the Poisson Equation is an iterative one, a lot of bookkeeping must be done to keep track of the marker particles, and the boundary condition for all the different possible configurations of the surface cells are very complex and time consuming. In addition, a very small grid spacing is needed to insure proper conservation of mass.

Numerical calculations for compressible flow are based on the same finite differencing methods as used for incompressible flow. However, the pressure calculation is somewhat simplified because the pressure of the gas is a strong function of the density and internal energy. Many times an ideal gas approximation will suffice to supply the functional relationships between the pressure, density, and internal energy. This strong functional relationship ties the continuity equation strongly to the momentum and energy balances. This strong

functionality aids iterative techniques that manipulate the pressure profile until the continuity equation is satisfied. This is exactly what the MAC method does for incompressible flow calculations via the Poisson Equation but appears less apparent.

General numerical methods that handle both compressible and incompressible flow calculations have been developed by combining the methods of the pressure calculations used in both types of flows. These methods manipulate the pressure profile until the continuity is satisfied. Two such methods are discussed by Pracht (1975) and Pakantar (1980).

The development of the numerical methods for multi-phase flow have capitalized on the development of these hybrid codes for incompressible and compressible flow. In fact, for the case of homogeneous flow such as considered here, very little modification would be needed to accommodate homogeneous flow calculations. Lyczkowski (1978) reviews the state of the art in numerical calculation in a multi-phase medium. In his review, he discusses the numerical algorithms of some of the promising numerical codes. Among those codes reviewed, mixed implicit-explicit algorithms were typical. In all cases, the pressure was treated implicitly by the same iterative methods discussed earlier to enforce the continuity equation. Typical explicit phases of the

algorithm were the viscous terms and the energy equation. The convective momentum terms were at times treated implicitly, depending on the algorithm. For the most part, convergence of the pressure profile requires the presence of the compressible phase. Lyczkowski's discussion is directed towards codes for the two-fluid model, as developed in Ishii (1975), which is the most complicated of the multi-phase models. Nonetheless, the characteristics of the codes discussed should apply for all the modeling regimes.

The numerical solution method used here to solve the equations of motion, describing the Vacuum Pan, is an extension of the work of Waldrop (1972) and Pitts (1976). This method was developed to model incompressible free surface flows in bays and estuaries. The solution method is explicit and avoids the difficulty of the implicit pressure solution via the Poisson Equation and the use of marker particles to locate the free surface. The vertical momentum equation is used directly to calculate the pressure profile explicitly, and the continuity relationship is used to locate the free surface. The basic calculation method originated from the work of Waldrop (1972). However, Waldrop's method of locating the free surface was not consistent with the overall mass balance, but Pitts (1976) extending Waldrop's work corrected the problem by applying the continuity

equation to locate the surface position.

The method uses a fixed inner grid system with a floating top cell. Because of its method of locating the free surface, the method can be made to conserve momentum, mass, and energy very easily. And as long as the range of surface levels are small, which is the case for some tidal variations for bays and estuaries, the technique performs very well. But when large volume changes occur, either the accuracy or the problem is extremely strained, because much of the volume is in the surface cells, or the solution cannot continue because the volume in one or more of the surface cells is negative. Although this sounds like a serious disadvantage over the MAC method, the advantages come because a very coarse grid spacing may be used and still locate the interface accurately while the MAC method requires a very small grid spacing. Other redeeming qualities of Waldrop's method are that it is much simpler and many times more efficient with computer time. Although it is true that incompressible free surface flow does not have complexities that two-phase free surface flow does, but, hopefully the solution method still applies.

But because Waldrop's method is explicit, one might expect to encounter problems with the multi-phase homogeneous flow calculations for fast transients. If such problems occur, consideration will have to be given

to doing some calculations implicitly or at least multi-step. Because of the structure of Waldrop's method, implicit or multi-step calculations may not eliminate the problems associated with the flashing transients of multi-phase flow problem.

However, for the prupose of this research it will be assumed that the explicit calculation will serve as an adequate solution method. The applicability of the Waldrop method will be discussed later as part of the purpose of this research.

While the method of the solution of the free surface problem developed by Waldrop (1972) and extended by Pitts (1976), will be used in this research, many modifications will have to be made to incorporate the two-phase nature of the problem. In addition, many of the finite difference methods as used by both Waldrop and Pitts were found to be completely inadequate. The most noticeable problem with Waldrop's and Pitt's codes is the improper differencing of the surface cells. Because the volume and boundary areas of the surface cells differ from the inner cells, these cells must be given special consideration. However, Pitts and Waldrop did not distinguish the surface cells from the inner cells, which leads to inaccuracies and instabilities in the numerical calculation. This problem will be eliminated with the discrete analogs derived in this

section. The derivation of the discrete analog will include the cell volume and boundary areas, thus, when the areas and volume change during the course of the simulation, the grid system can automatically compensate. Also, a subtle problem with the differencing methods of Pitt's and Waldrop's codes occurs when the convective terms are differenced. The subtle point is that traditional differencing methods cannot be blindly applied without considering the whole system of difference equations. Even though Pitt's and Waldrop's differencing methods for the convective terms are conservative, they are not consistent with the differencing of the other equations. In particular, the convection of momentum is not consistent with continuity equation. This point will be demonstrated later with the Well Stirred Tank (WSTRT) analogy and with an example that uses the discrete analog equations. As the result of this research, a philosophy was developed that gives clues that aid in the development of numerical techniques in general and especially when fluid convection is involved. Further development of the numerical code includes an implicit free surface calculation and a dynamic grid.

4.1 DEVELOPMENT OF THE PHILOSOPHY OF THE FINITE DIFFERENCE EQUATIONS

The mathematical development of the modeling equations presented in Chapter 3 were based on the continuum principles, but, because Finite Difference Equations are discrete, there will always be a degree of approximation in a numerical solution describing the spatial and time dependence of the solution set. This degree of approximation can be formally analyzed by a truncated Taylor series, as discussed in Roache (1976), to be approximately first order but approaching second order. However, a shadow of doubt can be thrown on this analysis, based on the experience with the development of this work and as discussed by Patankar (1980), as the sole basis to judge the difference equations. Therefore, the formal truncation error may be used as an indication of the accuracy but not the absolute rule to judge differencing techniques. Instead, there are many rules by which to judge a set of difference equations modeling a physical system. Since the continuum equations also reflect the conservation and transportation of mass, momentum, and energy, the numerical equations should, as much as possible, reflect the same properties. The significance of these properties as applied to the discrete equations are discussed below.

The conservative property as applied to Finite Difference Equations of conservation of mass, momentum, and energy, simply means the Finite Difference Equation, when summed, satisfies the integral of that conservative equation over some volume. Therefore, if a Finite Difference form is conservative over a cell volume, fluxes of the conserved quantity enter at the cell boundary. And, if the Finite Difference form is conservative over all the Finite Difference cells, the terms left after all the cells are summed are the overall material, energy, and momentum balances.

The importance of this property is obvious if accurate results are to be obtained. If the Finite Difference form is conservative, then there are no source terms (or generation) that are non-physical and only associated with the numerical form of the equations. This is not to say that numerically stable non-conservative forms are not acceptable but stable conservative forms would appear to be more desirable. Numerical stability and conservative property are related in that the conservative form places bounds on the total change of conserved species over the total volume in time.

The transportive property means that the convection terms transport disturbances in the direction of flow. The transportive property has physical significance like

the conservative property and the Finite Difference form should have this property to simulate the physical problem more realistically. But, for the Finite Difference form to convey disturbances in the direction of flow, there must be a logical check in the code to determine the direction of flow.

Based on the above discussion, physical reasoning must go into the design of a good code. The conservative and transportive properties may not be the most important for a particular problem and may be sacrificed for other properties based on physical reasoning. For example, conservative and transportive properties of Finite Difference may not be consistent with the accuracy of a spatial derivative of a conserved quantities at a certain point, and the conservative and transportive properties may not be as important for that calculation.

However, for this problem, the conservative and transportive properties are considered to be most important, and great care was taken to insure that these properties are exemplified in the code. The reasoning for this is that accurate evaporation rates of water and liquid level in the Pan are needed, therefore, the conservation of energy and mass is paramount. Furthermore, if the conservative property is not a characteristic of mass balance, the pan level cannot be predicted accurately, and since the boiling phenomena is highly sensitive to

pressure changes, the problem is literally unstable for non-conservative Finite Difference Continuity Equation forms. The significance of the transportive property may not be apparent, but, for most industrially important problems, convection is the most important mechanism to transport mass, momentum, and energy. Therefore, a non-transportive form may diffuse the natural convecting flow regime and destroy, for example, the vertical rise of hot liquid to the surface to be boiled off, thus, the physical nature of the problem would be destroyed.

Because of the importance of the conservative and transportive properties in the discrete equations, and in order to capitalize on a familiar concept, the development of the discrete analogs for the distributed conservative equations will be aided by the WSTRT analogy. This analogy gives a visualization of the proper forms of discrete equations, so they may be constructed so as to be conservative and transportive. Also, some of the mystique of the distributed equations is eliminated through this analogy.

Figure 4.1.1 is an idealized situation involving a WSTRT. The conservative equations can be written without much thought. To aid in the extension of this concept to multi-dimensions, Figure 4.1.2 is an illustration of a grid representation of the WSTRT system. In Figure 4.1.3, a two-dimensional Finite Difference grid, the blacken

dots indicate the center of the cell which is indexed in order to identify the cell, and the crossmarks represent the areas where inputs or outputs in mass, energy, and moemntum occur. Note the similarities between systems. The means to solve the WSTRT system are well known, therefore, solving the Finite Difference system should be analogous. The main problem in coding this WSTRT system is to determine if the mass flux of conservative quantity is an input or an output with regard to the cell and surrounding cells. This is simply taken care of with an algorithm for differencing the convective derivatives of conserved quantity. To complete the Finite Differencing of the conservative equations, the pressure and diffusion terms should also be differenced in a conservative fashion. If the viscous and compression forces are thought of as acting on the surface of the cell, a proper conservative scheme can be derived.

To place the analogy in a more mathematical plane, that will aid in the development of the Finite Difference Equations, especially when the dynamic grid is involved, a general property equation will be developed. This can then be used to describe the Finite Difference Equations for the dynamic grid. This general property equation is similar to the equation presented in Brodkey (1967), except the control volume will not be taken as moving

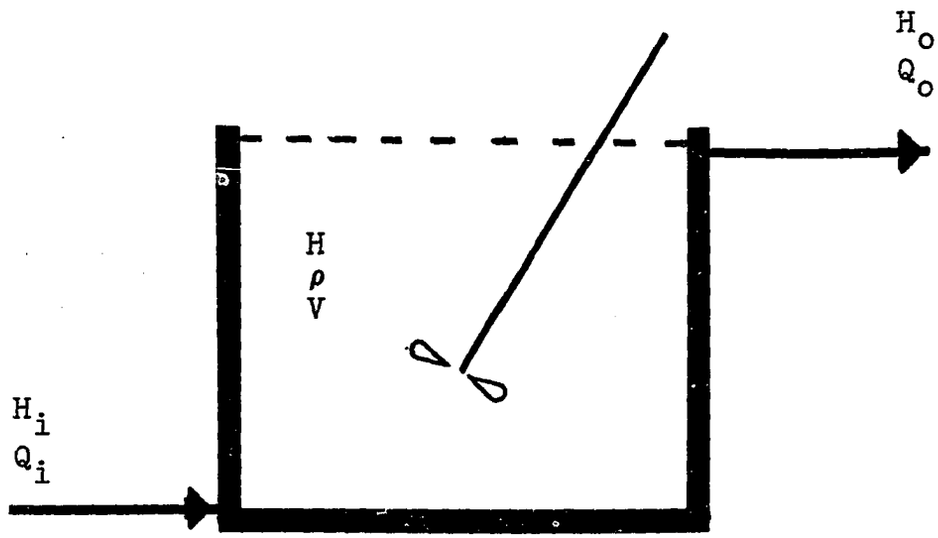


FIGURE 4.1.1 WELL STIRRED TANK

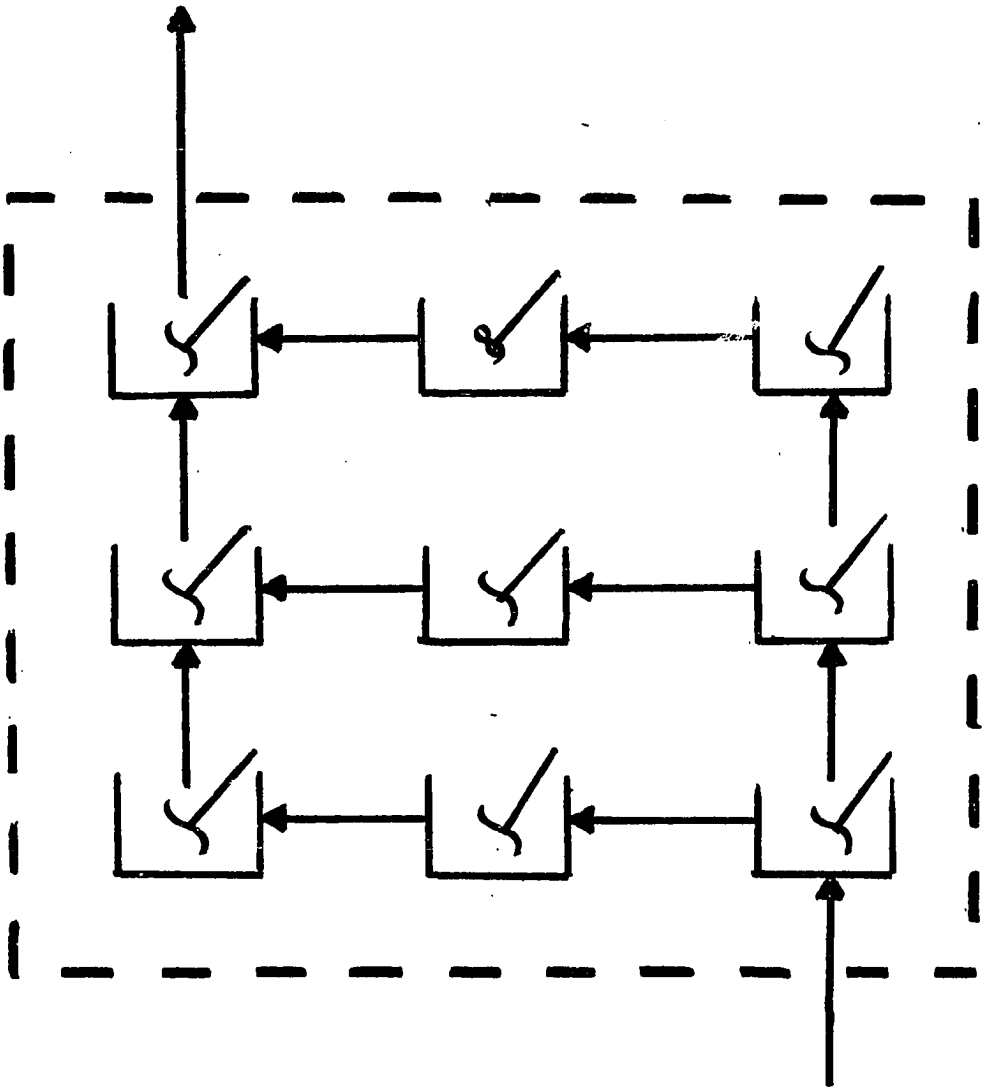


FIGURE 4.1.2 GRID REPRESENTATION OF WELL STIRRED TANK

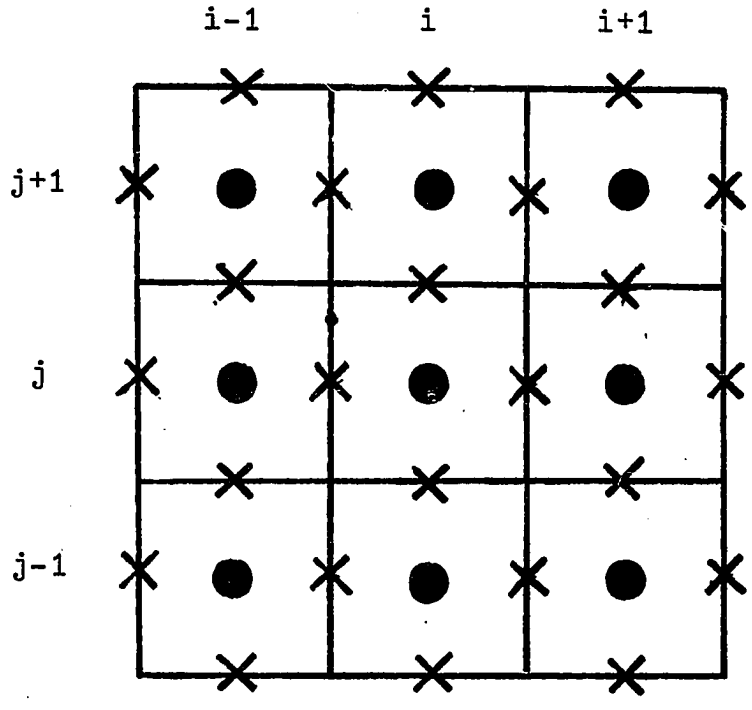


FIGURE 4.1.3 TYPICAL TWO-DIMENSIONAL FINITE DIFFERENCE GRID

with the fluid, which implies that the time derivative will not be a total derivative. However, the distinction between the total derivative and the partial derivative of the conservative species with respect to time for this equation is dubious. This is because the flux terms will contain the convection of the conserved species relative to the surface of the volume in consideration. Therefore, the meaning of the derivative will change with the magnitude of the velocity of the surface boundaries, two special cases, being the total or substantial derivative and the partial derivative. Equation 4.1.1 is the general property equation for the whole volume.

$$\frac{d}{dt}\int \rho \phi \, dV = - \oint \phi_F \cdot d\bar{A} + \int \phi_g \, dV$$

$$\phi_F = \rho U_{RB} \phi + \tilde{P} \qquad 4.1.1$$

The symbol ϕ is the general property per unit mass. The symbol ϕ_F is the sum of convection of the conserved species which crosses the cell boundary, plus, the terms which can be thought of as acting on the boundary or diffusing through the boundary. This function contains the viscous and compressive terms if ϕ is the specific momentum, and thermal conduction terms if ϕ is the specific enthalpy. The symbol ϕ_g is the generation of the general

property per unit volume.

Again, the analogy of the WSTRT is evident because the volume integrals can be thought of as the sum of the differential sized WSTRT cells. Remembering that if the sum of these small cells add to the total conservative general property equation for the total volume, the fluxes across each cell must cancel. Therefore, the discrete analogy of the fluxes should be constructed so that this is possible in the Finite Difference Equations. The volume terms, which are the accumulation of general property and its generation, which simply add as the integral suggests.

In order to derive the discrete Finite Difference Equations for each finite cell from the general property equation, the mean value theorem of calculus is used to arrive at the proper volume averages for the volume terms. The flux terms will be evaluated at the boundaries. Equation 4.1.2 is the discrete form of the general property equation as it applies to a cell in a Finite Difference grid. To avoid the problems associated with making a mathematically general statement, the discrete equation refers to the Finite Difference grid for the problem at hand, as shown in Figure 4.1.3. Furthermore, this discussion will be restricted to the two-dimensional case. Therefore, the discrete equation will refer directly to the Pan Proper and Free Surface. The

discrete models for the other sections can be arrived at through simple reasonings, based on the discussions here.

$$\frac{d}{dt}(\rho\phi\ V) = -\left((\rho u_{RB}\phi A)_{i+\frac{1}{2}} - (\rho u_{RB}\phi A)_{i-\frac{1}{2}}\right)_r$$
$$-\left((\rho w_{RB}\phi A)_{j+\frac{1}{2}} - (\rho w_{RB}\phi A)_{j-\frac{1}{2}}\right)_z + \phi_g V$$
$$-\left((\tilde{P}\ A)_{i+\frac{1}{2}} - (\tilde{P}\ A)_{i-\frac{1}{2}}\right)_r - \left((\tilde{P}\ A)_{j+\frac{1}{2}} - (\tilde{P}\ A)_{j-\frac{1}{2}}\right)_z \qquad 4.1.2$$

At this point, all the terms except the time derivative and the convections will be dropped, since the discussions to follow will not concern these terms. The discussions of these terms will be picked up later. Equation 4.1.3 is the resulting equation.

$$\frac{d(\rho\phi V)}{dt} = -\Delta_r(\rho u_{RB}\phi A) - \Delta_z(\rho w_{RB}\phi A) \qquad 4.1.3$$

As mentioned earlier, through general property equations, it is hoped that a way to incorporate the dynamic grid and construct the algorithm for the convective terms would be derived. Equation 4.1.3 contains a volume term, as well as boundary areas, which will be dynamic if the dynamic grid system is used. The convection terms are exactly as visualized by the WSTRT analogy, therefore, with the physical interpretation given by the

WSTRT analogy the proper algorithm can be constructed. Because of the way the numerical calculation proceeds, the time derivative will have to be split into its components. Equation 4.1.4 shows the result of the differentiation.

$$\rho V \frac{d\phi}{dt} + \phi \frac{d\rho V}{dt} = -\Delta_r(\rho u_{RB}\phi A) - \Delta_z(\rho w_{RB}\phi A) \qquad 4.1.4$$

The rate of change of mass in the cell is given also by the overall mass balance for the cell. Equation 4.1.5 is the discrete form of the mass balance derived by taking ϕ as one in Equation 4.1.3.

$$\frac{d\rho V}{dt} = -\Delta_r(\rho u_{RB}A) - \Delta_z(\rho w_{RB}A) \qquad 4.1.5$$

Equation 4.1.5 can then be used to eliminate the rate of change of mass in the cell from Equation 4.1.4. The resulting equation after rearranging the terms is Equation 4.1.6, because the subtraction is done before the multiplication computer truncation error is reduced.

$$\rho V \frac{d\phi}{dt} = -\Delta_r(\rho u_{RB}(\phi-\phi_i)A) - \Delta_z(\rho w_{RB}(\phi-\phi_i)A) \qquad 4.1.6$$

Equation 4.1.6 is the discrete analogy of the differential conservative equations in the form presented

by Bird, Stewart, and Lightfoot (1960), in which the continuity or mass balance has been eliminated. Equation 4.1.6 is a conservative discrete analogy in which the continuity relation has been eliminated but at the same time is mathematically satisfied.

The philosophical point is that the statement of conservation of momentum and energy involves the convection of mass, as does the mass balance or continuity equation. Therefore, the proper differencing method of the conservative equations must satisfy all the equations simultaneously. To make this point a little more clear, remember, for a WSTRT, when writing an energy balance, the mass balance is also involved, as shown by Equations 4.1.7 and 4.1.8. Therefore, the difference equations should use the proper difference forms so that the equations are not only conservative, in the sense that when all the equations are added the proper overall balances result, but also must locally be conservative or consistent with the mass balance for that cell.

$$\frac{dH\rho V}{dt} = \rho_i \, Q_i \, H_i - \rho_o \, Q_o \, H_o \qquad 4.1.7$$

$$\frac{d\rho V}{dt} = \rho_i \, Q_i - \rho_o \, Q_o \qquad 4.1.8$$

Equation 4.1.6 is conservative, if the property that is convected across the cell boundary is constructed consistently throughout the grid system. However, the transportive property is physically important, therefore, the WSTRT analogy must be invoked to arrive at the proper algorithm for the convection terms. Simply speaking, if the conserved property is an input, it is characteristic of the adjacent cell. Likewise, if the property is an output from the cell in question, it is characteristic of that cell. The upwind differencing algorithm presented in Roache (1976) accomplishes the WSTRT analogy. The algorithm is presented below in Table 4.1.1, with reference to Figure 4.1.4.

Only the radial term will be presented, since the vertical term is analogous. However, the mass rate leaving the top and bottom boundaries of the cell are calculated directly from the continuity equation. But the radial mass rate is assumed to be the linear average of the adjacent points. The algorithm is not exactly as presented by Roache, because of the way Equation 4.1.6 was derived. The algorithm presented in Roache was derived so that differencing would obey the transportive principle, which is exactly what has been accomplished through the WSTRT analogy.

Now that a consistent way to difference the

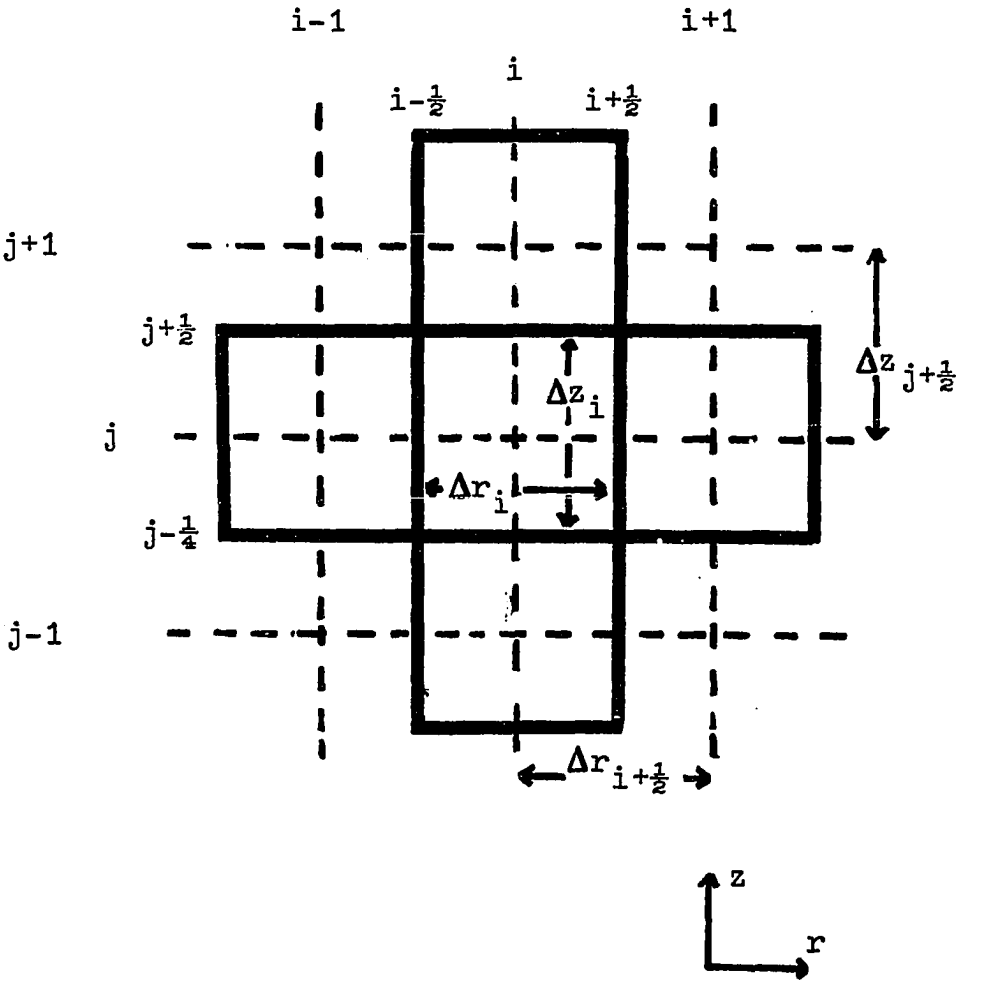


FIGURE 4.1.4 COMPUTATIONAL GRID CELL

TABLE 4.1.1: Upwind Differencing Algorithm

IF $uB = (\rho u_{RB} A)_{i-\frac{1}{2}} > 0$ $\quad \phi - \phi_i = \phi_{i-1} - \phi_i$

IF $uB = (\rho u_{RB} A)_{i-\frac{1}{2}} < 0$ $\quad \phi - \phi_i = 0$

IF $uF = (\rho u_{RB} A)_{i+\frac{1}{2}} > 0$ $\quad \phi - \phi_i = 0$

IF $uF = (\rho u_{RB} A)_{i+\frac{1}{2}} < 0$ $\quad \phi - \phi_i = \phi_{i+1} - \phi_i$

$$(\rho u_{RB} A)_{i-\frac{1}{2}} = \left[(\rho u_{RB} A)_{i-1} + (\rho u_{RB} A)_i\right]/2$$

$$(\rho u_{RB} A)_{i+\frac{1}{2}} = \left[(\rho u_{RB} A)_i + (\rho u_{RB} A)_{i+1}\right]/2$$

convective terms has been derived, the discrete form of the viscous, compressive, and body forces for the momentum equations shall be derived, as well as, the thermal diffusion terms for the energy equation. Because of the complexity of the viscous forces in their general form, the derivation of these terms will be omitted. Instead, the viscous forces will be taken directly from the modeling equation given in Chapter 3. The WSTRT analogy and Equation 4.1.2 will simply indicate that the diffusion terms should be differenced in a conservative fashion. The mathematical form of the viscous forces are given below in terms of the general property. These terms, of course, are differential diffusion forms of Equation 4.1.2 after dividing Equation 4.1.2 through by the volume, and then taking the limit, as the volume goes to zero. Equation 4.1.9 and 4.1.10 will serve as the definition of thermal diffusion also. Any discrete analogs for Equation 4.1.9 and 4.1.10 will, therefore, apply to the momentum equations as well as the energy equations.

$$D_{rr}(\phi) = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial \phi}{\partial r}\right) \qquad 4.1.9$$

$$D_{zz}(\phi) = \frac{\partial^2 \phi}{\partial z^2} \qquad 4.1.10$$

$$D_{\theta r}(\phi) = \frac{\phi}{r^2} \qquad 4.1.11$$

Both Equations 4.1.9 and 4.1.10 are differenced in a conservative form as shown in Equations 4.1.12 and 4.1.13 below.

$$D_{rr}(\phi) = (\rho_{i+\frac{1}{2}} A_{i+\frac{1}{2}} (\phi_{i+1} - \phi_i)/\Delta r_{i+\frac{1}{2}} - \rho_{i-\frac{1}{2}} A_{i-\frac{1}{2}} (\phi_i - \phi_{i-1})/\Delta r_{i-\frac{1}{2}}))/V_i \qquad 4.1.12$$

$$D_{zz}(\phi) = (\rho_{j+\frac{1}{2}} (\phi_{j+1} - \phi_j)/\Delta z_{j+\frac{1}{2}} - \rho_{j-\frac{1}{2}} (\phi_j - \phi_{j-1})/\Delta z_{j-\frac{1}{2}})/\Delta z_j \qquad 4.1.13$$

However, Equation 4.1.11 cannot be differenced in a conservative form because it looks like a source term, this is a problem that results from expressing the radial component of the stress tensor in the cylindrical coordinate system. Actually, mathematically, Equation 4.1.11 should cancel with the other terms for the inner cells if the overall momentum balance is to be observed. Since Equation 4.1.12 and 4.1.13 sum for the entire volume to give the stresses at the boundary, there might be some question as to why this should be included in the discrete analogy of the modeling equations.

Nonetheless, Equation 4.1.14 will be used as the discrete form of Equation 4.1.11 and used in programming.

$$D_{\theta r}(\phi) = \rho_i \frac{\phi_i}{r_i^2} \qquad 4.1.14$$

The generation term in Equation 4.1.2 is simply the body force for the vertical momentum equation. The discrete analog is Equation 4.1.15.

$$\phi_g V_i = \rho_i V_i \qquad 4.1.15$$

To complete the definition of the force acting on a cell, a discrete analog of the compressive forces must be stated. The radial gradient is approximated by Equation 4.1.16

$$\frac{\partial P}{\partial r} = ((P_{i+1} + P_i)\,\Delta z_{i+\frac{1}{2}} - (P_i + P_{i-1})\,\Delta z_{i-\frac{1}{2}})/2\Delta z_i \Delta r_i \qquad 4.1.16$$

The pressure gradient of the vertical direction is simply approximated by Equation 4.1.17.

$$\frac{\partial P}{\partial z} = \frac{P_{j+\frac{1}{2}} - P_{j-\frac{1}{2}}}{\Delta z_j} \qquad 4.1.17$$

The pressure along the vertical surfaces are not related to the grid points, because, the pressures will be calculated along the surface via the vertical momentum equation. This will be made clearer once the calculation sequence is outlined.

In the preceding discussions where the density is needed at the boundaries of the cell, this density is calculated simply by averaging the densities of the cells adjacent to the boundary. This applies in particular to Equation 4.1.12 and Equation 4.1.13.

4.2 NUMERICAL MODEL FOR VACUUM PAN

Now that the discrete analogs for the various terms presented in the modeling equations have been derived, the full set of numerical modeling equations will be presented and how the various modeling sections interact. The numerical modeling equations will be presented in the order that each equation for each modeling section supplies information to the calculation sequence. In summary, the calculation sequence is outlined below in steps (1) through (7).

(1) Calculate the radial velocity from the radial momentum equation.

(2) Calculate the enthalpy from the energy equation, then calculate the temperature and density.

(3) Rezone the grid system.

(4) Do any spatial averaging and integrate the overall balances, then calculate the mass fractions of components and spatial averaged physical properties.

(5) Calculate vertical mass fluxes and velocities from the continuity equation and also the vapor flux leaving the surface.

(6) Calculate the new surface position from the continuity equation.

(7) Calculate the pressure profile from the vertical momentum equation.

In the derivation of the discrete modeling equations, it was pointed out that a dynamic grid system could be used in conjunction with these equations. This dynamic grid system is important to the numerical solution because moving boundary problems are plagued with the problem of keeping track of the location of the boundaries. In particular, free surface problems such as the present modeling effort, where curvature of the surface and volume changes occur, a fixed grid system is inadequate.

Although Waldrop's method as extended by Pitts, has a floating top cell, the volume changes during the course of operation of the Vacuum Pan are large enough to strain the accuracy of the solution or produce negative cell volume. Therefore, the grid system will have to be dynamic to be compatible with the solution techniques for the whole operation of the Vacuum Pan. The easiest way to prevent the surface cells from running dry or expanding too large is to absorb some of the volume changes in the inner cells. This is the method that will be used to develop the dynamic grid used here. The forms of the discrete analogs of the modeling equations will not change because they were derived with the dynamic grid systems in mind.

Because the natural convecting flow in the Pan does not permit large deviations of the radial surface height from the average surface height, there is no need to distinguish differences in the inner cell vertical heights in the radial direction. Adjustments for curvature can be done with surface cells. Also, radial variation of the radial increments is an unneeded complexity. Therefore, varying the inner cell vertical heights with volume change so as to maintain a positive surface volume is all that is needed in the way of a dynamic grid. A better description of this dynamic grid system along with the calculations involved, are present as part of the outline of the calculation sequence for solving the numerical model. A more general discussion of the dynamic grid systems developed in the literature as well as the dynamic grid system used here is included in Chapter 6, Appendix III includes an example.

Each computational grid cell in the grid system is aligned such that the boundaries of the cell correspond to the physical boundaries of the Pan and the boundaries of each sectional portion of the Pan. This arrangement allows the boundary conditions to be easily applied and ensures that the conservative and transportive nature of each cell is characteristic of the computational space. The dynamic portion of the grid system is limited to the Pan Proper. Therefore, free surface must always be contained in the

Pan Proper.

4.2.1 RADIAL MOMENTUM

Taking the general property as the specific radial momentum, the equations for the modeled section can be derived. An explicit method is used to integrate these equations. The equations for the Pan Proper, Free Surface, and the Bottom are presented below. The equation for updating the radial velocity in the Bottom is a little different because the convective term can be evaluated implicitly.

a. Free Surface and Pan Proper

$$DUDT_{ij}^{n} = -\Delta_r^n\frac{(\rho u_{RB}A(u-u_i))}{\rho_i V_i} - \Delta_z^n\frac{(\rho w_{RB}A(u-u_j))}{\rho_i V_i}$$

$$-\frac{\Delta^n P}{\Delta r} + \nu D_{rr}^{n}(u) + \nu D_{\theta r}^{n}(u) + \nu D_{zz}^{n}(u) \qquad 4.2.1$$

$$u_{ij}^{n+1} = u_{ij}^{n} + (DUDT_{ij}^{n} + DUDT_{ij}^{n-1})\Delta t/2 \qquad 4.2.2$$

b. Bottom

$$u_7^{n+1} = u_7^n - \frac{PBIP1 - PBIM1}{\rho_7 \Delta r}\Delta t - (u_7^{n+1})^2 c_2$$

$$(u^{n+1})^2 \approx u^{n+1}u^n$$

$$c_2 = \Delta(\tfrac{1}{r})/\Delta r^2 \Delta t\, r_7^2\, 2$$

$$u_7^{n+1} = u_7^n - \frac{1}{\rho}\frac{\Delta P}{\Delta r}/(1+c_2 u^n)\Delta t \qquad 4.2.3$$

4.2.2 ENTHALPY, TEMPERATURE, AND DENSITY

The energy equation, like the radial momentum, is solved explicitly via the equation below. The equations for the Pan Proper and the Free Surface will be lumped together again, but remember, the flux of energy leaving the surface is the result of vaporization. The flux of vapor leaving the surface cell will be calculated later, as will be outlined momentarily. Heat is transfered into the Pan in the Calandria. This flux of energy is given the symbol ECOEFF, this flux is the evaporation coefficient mentioned in Chapter 3. Feed is introduced into the Bottom and effects the enthalpy balance for the Bottom.

a. Free Surface and Pan Proper

$$DHDT^{n}_{ij} = -\Delta^{n}_{r}\frac{(\rho u_{RB} A(H-H_i))}{\rho_{ij} V_{ij}} - \qquad 4.2.4$$

$$\Delta^{n}_{z}\frac{(\rho w_{RB} A(H-H_j))}{\rho_{ij} V_{ij}} + \alpha D^{n}_{rr}(T) + \alpha D^{n}_{zz}(T)$$

$$H^{n}_{ij} = H^{n}_{ij} + DHDT^{n}_{ij}\Delta t \qquad 4.2.5$$

b. Calandria

$$DHDT_j^n = -\frac{\Delta_z^n(\rho w_{RB}(H-H_j))}{\rho_j \Delta z} +$$

$$ECOEFF\ POA/\rho_j + \alpha D_{zz}^n(T) \qquad 4.2.6$$

$$H_j^{n+1} = H_j^n + DHDT_j^n \Delta t \qquad 4.2.7$$

c. Bottom

$$DHDT^n = ((-\rho wAH)_1 - (\rho wAH)_2 + F\ HF)/\ V$$

$$H^{n+1} = H^n + DHDT^n \Delta t \qquad 4.2.8$$

Once the enthalpy is calculated, the density of the mixture is calculated by checking to see if the enthalpy is large enough to suggest that the vapor phase is present. This is done by calculating the mixture temperature, Equation 4.2.9.

$$T = H / CP \qquad 4.2.9$$

If the temperature is greater than the boiling point of the mixture, given by Equation 3.4.16, then the vapor phase is present.

$$TBOIL = f\ (P) + BPE \qquad 3.4.16$$

Of course, if the vapor phase is present, then the temperature of the mixture is at the boiling point. The mass fraction of the vapor is then calculated by Equation 3.4.13.

$$XV = \frac{H - HL}{HV - HL} \qquad 3.4.13$$

The liquid enthalpy and vapor enthalpy functional relationships are given by Equations 3.4.10 and 3.4.11, respectively. The density of the mixture is then calculated by Equation 4.2.10.

$$\frac{1}{\rho} = \frac{1-XV}{\rho V} + \frac{XV}{\rho LS} \qquad 4.2.10$$

The vapor density is given by Equation 3.4.3, which is corrected for changes in pressure relative to the reference pressure. The liquid and solid mixture density (ρLS) is given by Equation 3.4.6. The liquid density is given by Equation 3.4.5. The calculation of mixture enthalpy does not adjust the local mass fractions

when vaporization occurs, as discussed earlier.

$$\frac{1}{\rho LS} = \frac{1-XCP}{\rho L} + \frac{XCP}{\rho C} \qquad 3.4.6$$

4.2.3 DYNAMIC GRID

In order to track the volume change in the Pan and maintain a positive volume in the surface cells, for a fixed number of cells, it is necessary to adjust the grid positions. Adjustments are made only in the vertical direction. Figure 4.2.1 is an illustration of a typical grid arrangement. As is shown in the Figure, the inner cell vertical and radial cell widths are equal, but the surface cell heights may differ as a function of the fluid dynamics. The adjustments will be done by expanding or contracting the inner cell heights, as the average height of the fluid above the Calandria and Downtake changes. The average height is calculated by adding the average surface cell height to the sum of the inner cell heights. The rate of change of the inner cell heights are then calculated by Equation 4.2.11. Exponential smoothing is used to give a smooth rate of change.

$$\text{SURFDT} = \left(\left(\bar{h} + \text{jmax DZ} \right)^{n} - \left(\bar{h} + \text{jmax DZ} \right)^{n-1} \right) / \Delta t / \text{jmax} \qquad 4.2.11$$

$$\text{DDZDT}^{n+1} = \text{DDZDT}^{n} - (\text{DDZDT}^{n} - \text{SURFDT})\ \text{THETAS} \qquad 4.2.12$$

$$0 \leq \text{THETAS} \leq 1$$

Once the rate of change of the inner cell heights is found, the cell height is updated by Equation 4.2.13.

$$DZ^{n+1} = DZ^{n} + DDZDT^{n+1}\Delta t \qquad 4.2.13$$

The dynamic grid acts as a musical accordion, expanding or contracting according to the volume of fluid inside the Pan. Because the grid system is dynamic, each grid cell center may be moving. The continuity equation will be used to calculate the flux of mass in or out of the top cell boundary, but if the absolute value of the vertical component of the fluid velocity is to be extracted for this mass flux, given the fluid density, the vertical velocity of the cell boundary must be known. Likewise, if the vertical fluid velocity at the cell center is to be calculated, the velocity of the cell center must be known. Since the vertical velocity of the fluid at the cell center is needed for the vertical momentum equation, the cell center velocity will be calculated by Equation 4.2.14.

$$DPDT_{j} = DDZDT(2j-1)/2 \quad j=1,2...jmax \qquad 4.2.14$$

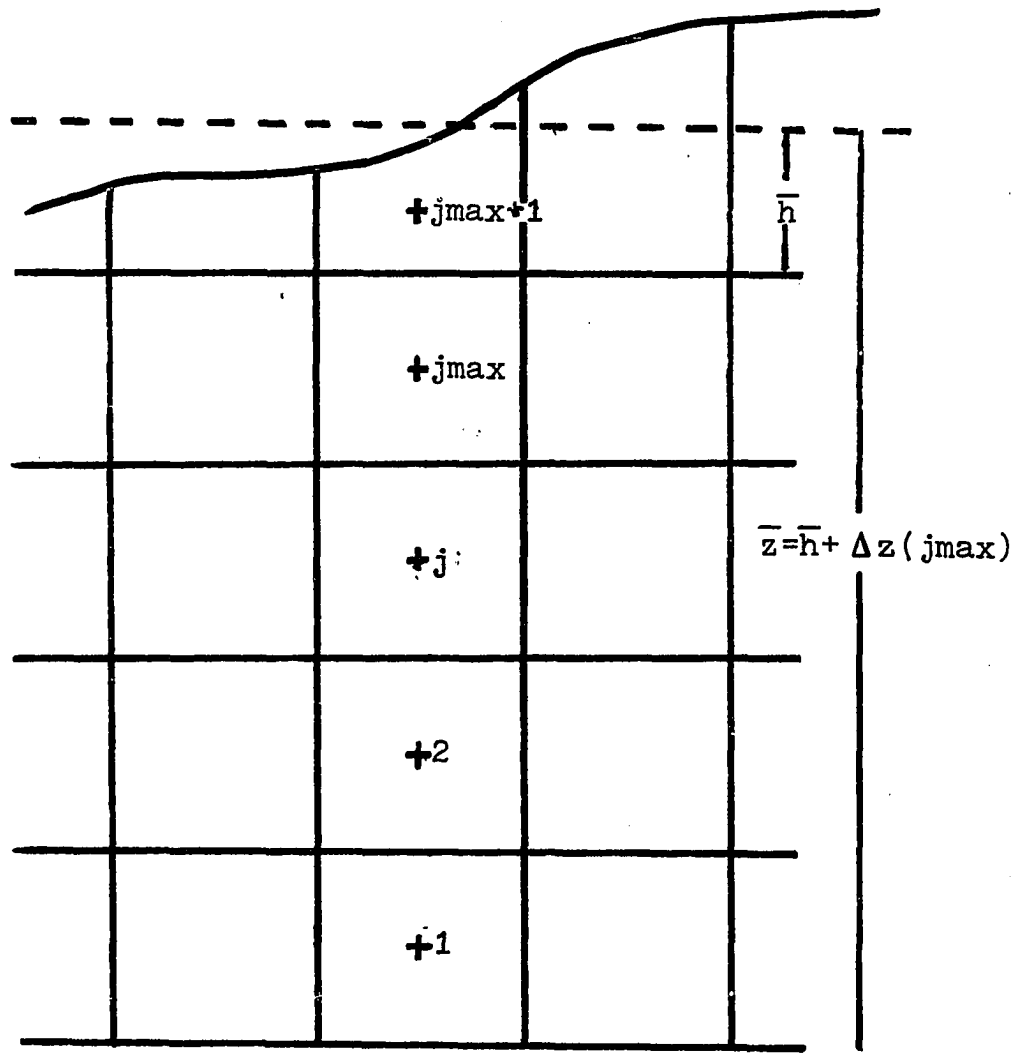


FIGURE 4.2.1 TYPICAL GRID ARRANGEMENT

4.2.4 OVERALL BALANCES

The mass fractions of the components in the Vacuum Pan are calculated via the overall mass balances. These mass fractions are then used to calculate physical properties needed for the other calculation steps. Those physical properties being the heat capacity, as given by Equation 3.4.9, the viscosity of the mixture, as given by Equation 3.4.17 and 3.4.18, the enthalpy of the vapor, Equation 3.4.11, and the density, Equation 3.4.1.

Because the dynamics of these equations are slow compared to the distributed balances of mass, momentum, and energy for each cell, the integration time step will be limited by the distributed balances. It would therefore, be possible to integrate the overall equation in the numerical code at a different time step. However, this was not done and the overall equations were integrated with a very small time step. Since such a small integration step is used, the integration method is not very important. The integration method that is used in the program is simply a one step forward time integration. The time derivative is calculated from the latest values of the inputs and outputs available. Again, whether the old or new inputs or outputs were used is not important, since the time step that will be used is very small.

4.2.5 VERTICAL VELOCITY AND MASS FLUX LEAVING THE CELL

The vertical velocity and mass flux leaving the cell are calculated algebraically by the continuity expression, once the volume, density, and radial velocity of each cell are known. Of course, these are given by the previous explicit calculations. The continuity relationship, also, applies at the top cell but, this is a special case by which the surface position is located, this will be discussed later. Once the pressure drop occurs across the Bottom, from the Downtake to the Calandria, the radial flow plus feed into the Bottom is converted into vertical flow in the Downtake and Calandria. Equation 4.2.15 is the continuity relationship for the top of the Downtake, Bottom of the Downtake, and radial flow at the Bottom, plus the feed into the Bottom. Figure 3.3.1 will help in the understanding of how the Downtake, Bottom, and Calandria is divided.

$$A_1 w_1 = A_2 w_2 = -A_7 u_7 \qquad 4.2.15$$

Likewise, the continuity relationship for the Calandria entrance is given by Equation 4.2.16. Equations 4.2.15 and Equation 4.2.16 add together to give Equation 3.3.20, the overall continuity relationship for the Bottom and Downtake.

$$A_5 w_5 = A_7 u_7 + F/\rho_7 \qquad 4.2.16$$

The direction of flow is always limited to be in the positive or counterclockwise direction, down the Downtake and up the Uptake (Calandria). Equation 4.2.16 is the boundary condition for the Calandria continuity relationship, which is Equation 3.3.5.

The mass flux at each cell boundary in the Calandria is given by Equation 4.2.17 and the velocity at the center of each cell is given by Equation 4.2.18.

$$(\rho w)_{j+\frac{1}{2}} = (\rho w)_{j-\frac{1}{2}} - \frac{\Delta \rho}{\Delta t} \Delta z \qquad 4.2.17$$

$$w_j = 0.5\ ((\rho w)_{j+\frac{1}{2}} + (\rho w)_{j-\frac{1}{2}})/\rho j \qquad 4.2.18$$

With the mass flux up the Calandria and the mass flux down the Downtake calculated, the calculation proceeds into the two-dimensional Pan Proper. The mass flux relative to the cell boundary is calculated by Equation 4.2.19.

$$(\rho w)_{j+\frac{1}{2}} = (\rho w)_{j-\frac{1}{2}} - \frac{\Delta_r(\rho u_{RB} A)}{A_z(i)} + \frac{\Delta(\rho_i V_i)}{\Delta t\ A_z(i)} \qquad 4.2.19$$

The velocity at the cell center is calculated by Equation 4.2.20. Notice that the velocity of the fluid at the cell center is adjusted by the velocity of the cell center. This is the result of the dynamic grid system.

$$w_j = 0.5\ ((\rho w)_{j+\frac{1}{2}} + (\rho w)_{j-\frac{1}{2}})/\rho_{ij} + DPDT_j \qquad 4.2.20$$

The calculation proceeds upward, increasing in vertical height, above the Calandria and Downtake, until the cell just below the surface cell is reached. The mass flux of vapor leaving, if any, from the top cell is then calculated by Equation 4.2.21.

$$E_i = \rho V(w_v - w_s) = W_V^* \gamma \qquad 4.2.21$$

As discussed earlier, Equation 4.2.21 is the semi-theoretical relationship, describing the slip velocity of vapor relative to the liquid. However, because of lack of experimental data, Equation 4.2.21 is simply used as a method to remove the vapor present in top cell.

4.2.6 SURFACE POSITION

The height of each surface cell is calculated by a mass balance, therefore, the equation is just a continuity relationship. The surface equation is the same continuity relationship used in the grid cells below the surface to calculate the vertical velocity of the cell center and the mass flux leaving the top cell boundary. Because the mass flux of vapor has been already calculated by Equation 4.2.21 the equation can be used to calculate the rate of change of mass in the cell, and thus, with the density known, the surface height. Equation 4.2.22 is the Finite Difference Surface Continuity Equation. The last term in the equation is used to supply surface smoothing needed for stability.

$$(h\rho)_i^{n+1} = (h\rho)_i^n - \frac{\Delta_r^n(\rho u_{RB}A)}{A_z(i)} + (\rho w_{RB})_{jmax+\frac{1}{2}} \quad 4.2.22$$

$$- E_i + SFSMTH\ D_{rr}(h)$$

As can be readily seen, Equation 4.2.22 is in tri-diagonal form, therefore, an implicit solution of the surface height is possible. This is a convenience afforded only to two-dimensional problems. If the model was three-dimensional, iterative solution techniques would have to be used. If the equation was solved explicitly, the equation without the diffusion term would

be unstable because central difference equations, like Equation 4.2.22, are unstable when integrated as demonstrated in Roache (1976). Surface diffusion or smoothing in the explicit formulation adds feedback between the grid points to stabilize the equation.

However, the amount of smoothing needed for stability of the explicit formulation is large and therefore, the free surface does not respond adequately to the fluid dynamics. Formulating an implicit solution eliminates the stability problems associated with the form of the difference equation but, because the other terms in the equation are affected by the surface position but are predicted explicitly, some surface smoothing is needed to insure stability. It was found by experiment, that for stability, the surface diffusivity needs to be greater than 0.1 FT./SEC.^{2}. The implicit surface diffusivity is at least a thousand times smaller than the surface diffusivity needed to stabilize the explicit calculation. A nominal surface diffusivity of 2.0 FT./SEC.^{2} was used for all numerical calculations with the implicit surface calculation.

The tri-diagonal algorithm is presented in the computer code. Basically, it is the code developed by Roache (1976).

Once the new surface cell height has been calculated, the velocity of the center of the surface cell can be

calculated by Equation 4.2.23.

$$w_{jmax+1} = ((\rho w_{RB})_{jmax+\frac{1}{2}} - \frac{\Delta_r(\rho u_{RB} A)}{2 A_z(i)}$$

$$- \frac{\Delta\rho V_i}{2\Delta t\ A_z(i)})/\rho_{jmax+1} + DPDT_{jmax+1} \qquad 4.2.23$$

$$DPDT_{jmax+1} = \frac{\Delta h}{2\Delta t} + DDZDT(jmax+1)$$

The velocity of the surface may be calculated if needed for plotting by Equation 4.2.24.

$$w_s = \frac{\Delta h}{\Delta t} + DDZDT(jmax) \qquad 4.2.24$$

4.2.7 PRESSURE CALCULATION

At this point, all the variables in the solution matrix have been calculated except the pressure profile. The pressure profile can be calculated from the vertical momentum equation. Although, the hydrostatic approximation is going to be used in the program, the full vertical momentum equation will be Finite Differenced in the same conservative fashion as the other equations for the sake of completeness. The hydrostatic head approximation can then be derived by eliminating all the terms except the body forces and the pressure gradient. The exceptions to this rule apply in the Downtake and Calandria where the friction pressure drop is also retained. The pressure calculation starts at the surface cell because the pressure at the surface is known. The difference equation allows the pressure on the lower boundary of the surface cell to be calculated. The pressure at the cell center is then the linear interpolation of the pressure difference from the top to the bottom boundary of the cell. Figure 4.2.2 illustrates this point. Once the pressure for all the cells along the surface has been calculated, the calculation can be proceeded to the next grid level below. Repetitively, the calculation then proceeds from the free surface to the Bottom of the Pan. The pertinent difference equations

for each section are presented below.

The pressure across the upper boundaries of the Downtake and Calandria are taken as the area average of the pressure forces on their surfaces. While the Calandria is treated in a distributed fashion, the Downtake is taken as one lump. The two pressures calculated at the lower boundary of the Downtake and Calandria are fed back into the Bottom Momentum Equation at the next time step. Likewise, the radial pressure profiles in the Pan Proper and Free Surface are used in their respective Radial Momentum Equations. Thus, the calculation sequence has been cycled.

a. Free Surface and Pan Proper

$$\rho_{ij}\frac{\Delta w_{ij}}{\Delta t} + \frac{\Delta_r(\rho u_{RB}(w-w_i))}{V_{ij}} + \frac{\Delta_z(\rho w_{RB}(w-w_j))}{V_{ij}} \qquad 4.2.25$$

$$= -\frac{\Delta P}{\Delta z} + \nu D_{rr}(w) + \nu D_{zz}(w) + \rho_{ij}$$

$$P_c = P_u - \frac{\Delta P}{\Delta z}\Delta z/2$$

b. Downtake

$$PBIM1 = PNUP + DPFR + TUBEH\,\rho + \rho\frac{\Delta w}{\Delta t}TUBEH \qquad 4.2.26$$

$$DPFR = 8\,\mu w_1 TUBEH/R^2_{dwn} \qquad 3.3.22$$

$$PNUP = \frac{\Sigma P_i A_i}{\Sigma A_i}$$

c. Calandria

$$\rho \frac{\Delta w}{\Delta t}_j + \frac{\Delta_z(\rho w_{RB}(w-w_j))}{\Delta z} = - \frac{\Delta P}{\Delta z} + FR + \rho_j \qquad 4.2.27$$

$$FR = 32 \rho_j \nu w / D_t^2 \qquad 3.3.8$$

$$PNUP = \frac{\Sigma P_i A_i}{\Sigma A_i}$$

If desired, the action of a pump in the Downtake or Bottom may be simulated by simply increasing the pressure drop across the Downtake to the Calandria by the amount of head supplied by the pump.

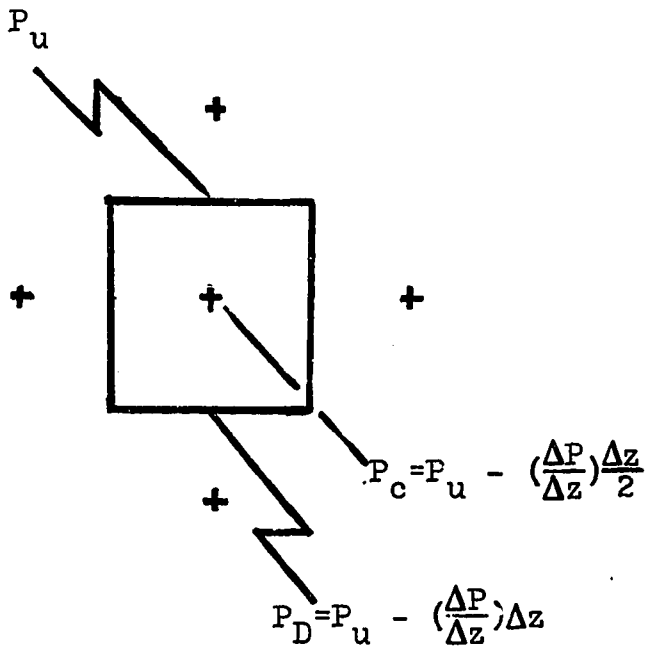


FIGURE 4.2.2 DIFFERENCING VERTICAL PRESSURE GRADIENT

CHAPTER 5

RESULTS

In the previous chapters a mathematical model of the Vacuum Pan Sugar Crystallizer was developed. The model includes overall material balances to simulate the effect of feed input, evaporation, and crystal growth on Pan operation. The distributed mass, momentum, and energy equations are included to simulate the distributed nature of the Pan operation. The model is capable of simulating the operation of a typical Industrial Calandria Vacuum Pan during the later periods of its operation, when vigorous boiling does not occur. This limitation results from instabilities in the numerical solution method when vigorous boiling occurs, vigorous boiling is characteristic of the early periods of the batch. In terms of the utility of the model this is not a severe limitation.

In the following pages, sensitivity of the numerical solution will be demonstrated to the thermal diffusivity and kinematic viscosity, and to Pan design and operating conditions. The sensitivity of the solution to the thermal diffusivity and kinematic viscosity demonstrates that convection is the most important mechanism to transport momentum and energy. The sensitivity of studies varying Pan design and operating conditions demonstrate the utility of the model as a research tool to aid in design

of Vacuum Pans, design of control systems for Vacuum Pans already existing or in the design stage. The significance of the model is its ability to calculate local supersaturation and growth rate profiles and velocity profiles in the Pan. The interaction of these velocity and growth rate profiles contributes to the increase of the variance of the crystal size distribution (CSD), and excessive local supersaturation contributes to unwanted nucleation occurring. In all cases, the model simulations demonstrated that significant growth rate profiles exist in the Vacuum Pan. The effect of these profiles quantitatively cannot be demonstrated until a distributed particle population balance is integrated with the fluid dynamics. These studies will also demonstrate how various designs and operating conditions affect these profiles as well as the velocity profiles and other pertinent Pan statistics. But since heat transfer correlations for the tubes do not exist that are sensitive to Pan design and the operating conditions, sweeping statements concerning Pan performance cannot be made. Future versions of the model will include more realistic heat transfer correlations. Comparisions of the predicted Calandria tube velocity from these studies against data in the literature shows favorable results.

Concluding this chapter, numerical difficulties with the solution method are discussed as well as the

applicability of the hydrostatic head assumption for modeling natural convection and boiling in the Vacuum Pan.

The methodology for performing the sensitivity studies mentioned above is as discussed below. The numerical integration is started at various operating points and the numerical model is allowed to come to a steady state. This steady state is accomplished by feeding water into the batch to match exactly the evaporation rate, maintaining constant heat input, and specifying the volume fraction of crystal and not allowing it to change, then integrating the dynamic model until the fluid dynamic transients disappear. The volume fraction crystal is maintained constant by artificially setting the calculated growth rate to be zero. Doing the simulation in this fashion causes the overall balances of sucrose, impurities, and water to maintain the same mass fractions as the initial conditions. This allows the perturbation of certain conditions while keeping others constant, thus, a true partial derivative is obtained. This type of analysis is justified for the crystallizer, when two-phase transients do not exist, because the fluid dynamics of the Pan are fast compared to the growth of crystals and the change of volume in the Pan.

5.1 SENSITIVITY OF CALCULATION TO THE KINEMATIC VISCOSITY AND THERMAL DIFFUSIVITY

One of the assumptions in the derivation of the model was the absence of excessive turbulence, that is, that laminar flow conditions exist. Thus, the need for turbulence models for this type of flow has not been explored. However, it is understood that in reality there is turbulent mixing in the Pan, especially when boiling occurs. During operation of the Pan, when boiling is not occurring, the laminar flow assumption is certainly valid because the viscosity of the mixture in the Pan is forty to five-hundred times the viscosity of water, while the velocities in the Pan are most of the time less than 1 FT./SEC.. Because of the uncertainty about the two-phase flow phenomena, experiments were run at various levels of viscosity and Prandtl number to test their effect on the profiles in the Pan Proper. The experiments demonstrate that the effects of the Thermal Diffusivity and Kinematic Viscosity over reasonable ranges of values are not significant. Table 5.1.1 is a log of the experimental runs. Velocity profiles for these runs are presented in Appendix II. These velocity profiles are plotted on one-half of an axisymmetrical cross-section of the Pan. The arrows indicate the magnitude and direction of the fluid velocity. For

convenience, the base of the arrow is located at the grid point and the radial and vertical velocity components are added to give the vector plotted.

Referring to Table 5.1.1, the first case and its corresponding figure presents typical conditions in the Vacuum Pan. All the other cases are perturbations of the first case to demonstrate the effect of the Thermal Diffusivity and the Kinematic Viscosity. In Cases 1 - 8 the effect on the velocity profiles is small. The last case, (case 9) is only included to indicate how large the diffusivities would have to be increased before the solution is effected. In fact, the Thermal and Momentum Diffusivity used in this case are in the range of liquid metals. Cases 2 and 3 in Table 5.1.2 also have special computational significance, since both the Thermal Diffusivity and the Kinematic Viscosity are zero. The significance of these cases will be discussed in Chapter 7. Therefore, as expected for the crystallizer, as in most industrial problems, the convective terms are the most important mechanism to transport momentum and energy. Extensive data about the experiment was omitted, because small changes in the velocity profiles presented in the figures are synonymous with small changes in all of the properties characterizing the experiment.

TABLE 5.1.1: LOG OF MODEL RUNS VARYING THE THERMAL AND MOMENTUM DIFFUSIVITIES

CASE	THERMAL DIFF. ($FT^2/SEC.$)	KINEMATIC VIS. ($FT^2/SEC.$)	PRANDTL NO.
1	1.34×10^{-6}	2.68×10^{-3}	2000
2	0.0	2.68×10^{-3}	
3	0.0	0.0	
4	1.34×10^{-4}	1.34×10^{-2}	100
5	1.34×10^{-6}	1.34×10^{-6}	1
6	1.34×10^{-6}	1.34×10^{-4}	100
7	1.34×10^{-4}	1.34×10^{-4}	1
8	0.0	1.34×10^{-4}	
9	1.34×10^{-4}	2.68×10^{-1}	2000

5.2 EFFECT OF PAN DESIGN AND OPERATING CONDITIONS

The design and operating conditions, as pointed out in Hugot (1972) and Honig (1963), have a profound effect on the quality of the CSD produced and the batch time needed to produce a desired crystal size. The importance of a large downtake and large tube diameters is stressed in order to reduce the resistance to recirculating flow. However, increased tube diameter and downtake diameter cause decreased heat transfer area. The heat load is, of course, the forcing function causing the recirculation to occur. Hugot attempts an optimization to find the pan design that minimizes the resistance to flow. Although his method of analysis is correct, he was not able to include the effect of pan design on the fluid dynamics and assumed the recirculating flow rate was constant between pan designs. The model developed here, offers an alternative method of analysis which is more realistic. Obviously, considering the design variables in combination with the variety of operating conditions, finding an optimal Pan could be difficult. But, if judicious engineering constraints are applied the basic characteristics of a good circulating Pan can be determined. Good recirculation is synonymous with a good Pan because good recirculation promotes good heat transfer and a reduced effect of growth variation on

the CSD. The model offers an inexpensive way to accomplish such a characterization by studying the effect of varying Pan design and operating conditions. This leads into the discussion of the effects of the operating conditions and Pan design to demonstrate the model applicability for such studies.

Presented in Table 5.2.1 are a few typical design variations of industrial pans. Table 5.2.2 summarizes a series of experiments using the model to simulate these typical pans under various operating conditions. Table 5.2.3 summarizes the results of these experiments varying the design of the pan, volume fraction crystals, heat flux in the tubes, level of the pan, supersaturation, and pan pressure. As can be seen from Table 5.2.1, four different pans were simulated. Pan A and Case 1 will be used as the base case for discussion. In the following paragraphs the effect of pan design will be discussed first and then the operating conditions. Cases 1, 3, 8, and 10 will demonstrate the effect of pan design, comparing Pan A against Pans B, C, and D. Cases 1, 2, and 9 will demonstrate the effect of pan level. Cases 1 and 4 will demonstrate the effect of the presence of crystals. Cases 1, 4, 6, and 7 will demonstrate the effect of heat load and the interaction with crystal content. Cases 1, 5, and 11 will demonstrate the effect of pressure and the interaction with supersaturation. Case 12 against all the other cases will demonstrate the

effect of lower purity batch. Figures 5.2.1 (1) - (12) are the velocity profiles for the cases. Figures 5.2.2 (1) - (12) are the growth profiles for the cases.

The construction and meaning of the velocity profiles in Figure 5.2.1 are the same as discussed earlier. The growth rate profiles, Figure 5.2.2, are plotted on the same axisymmetrical half-section view of the Pan. For convenience, these profiles are indicated by an integer scale rather than an absolute magnitude. The integer representing the growth rate is calculated by the following formula after truncating the decimal.

$$\text{INTEGER} = (9)\left(\frac{\text{GROWTH RATE - MIN. GROWTH RATE}}{\text{MAX. GROWTH RATE - MIN. GROWTH RATE}}\right)$$

The scale thus includes the integers zero to nine.

Case 3 (Pan B), differs from Case 1 (Pan A), only in the diameter of the Downtake. Referring to Table 5.2.3, the effect of reducing the Downtake diameter was to slightly reduce the recirculation rate and increase the variance of the supersaturation. A reduction in recirculation can only be viewed as detrimental to CSD.

Case 8 (Pan C), is a variation of Case 1 (Pan A), in several aspects, Pan C's Calandria diameter is smaller than the Pan Proper diameter, and the tubes are shorter, three feet long, and smaller, four inches in diameter. The effect on the velocity profiles is drastic,

completely changing the circulation pattern. This is illustrated by comparing Figures 5.2.1 (1) and (8). The changing flow pattern is basically caused by the difference in Calandria diameter and the major diameter of the Pan. As shown in Table 5.2.3, the recirculation is lower and the variance of the supersaturation and the difference between maximum and minimum supersaturation are larger for Case 8. Therefore, Pan C is not superior to Pan A.

Case 10 (Pan D), is designed to demonstrate the effect of an extra large Downtake but at the expense of heat transfer area. The trade off is not a superior choice over Pan A for the same reason as the previous case.

The level at which a batch is terminated is often the concern of pan designers when considering optimization of the batch cycle time. The higher the level in the Pan, the more sugar can be produced. However, there are practical limits to this line of reasoning that are obvious, but there are other ones that may not be quantified without a model that is sensitive to the effects of the hydrostatic pressure or level of the Pan in reducing circulation through the tubes. Pressure in the tubes increases as the level rises, if the pressure is high enough no boiling will occur in the tubes. If no boiling occurs, the driving force for

recirculation is reduced to a low level. Referring to Tables 5.2.2 and 5.2.3, the break between fast recirculation and slow may be quick as the level rises, as evidenced by the abrupt change in recirculation between Cases 2 and 9, while little change in recirculation rate occurs between Cases 9 and 1. Oddly enough, Case 2, with lower level had a greater volume average variance of the supersaturation. The effect of this small increase in the volume averaged variance of Case 2 over Case 1 is not significant in itself except when one considers that the recirculation rate of Case 2 is twice that of Case 1. This result seems to be contrary to what the literature suggests should happen. This is another example of conditions in the Pan that cannot be predicted without a distributed model. Viewing Figures 5.2.1 (1) amd (2), one can see that the velocity profiles are completely different. Likewise, the growth profiles Figures 5.2.2 (1) and (2), are also different. The effect of the level on the circulation and growth patterns in the Pan Proper is the result of more vapor in this section, caused by a higher heating rate per amount of material in the Pan at that time.

The effect of the volume fraction of crystals in the Pan is demonstrated between Cases 1 and 4. As can be seen by comparing the recirculation rates for each case in Table 5.2.3, the experiment with no crystals which is

characteristic of early time intervals of Pan operation has a much higher recirculation rate. The decreased recirculation caused by the presence of the crystals, Case 1, is caused primarily by three factors. The increase of the volume fraction crystals increases the pressure in the tubes due to a higher average density, displaces the liquid which thermally expands with increasing temperature by a crystal that does not expand with increased temperature, and increases the viscosity, all of which restricts recirculation.

Because correlations for heat transfer coefficients are not available for the local conditions in the tube of Vacuum Pan Sugar Crystallizers, as discussed earlier, typical values of the heat flux were calculated based on steam consumption per heat transfer area. To demonstrate the effect of heat load on the Pan, Cases 6 and 7, which are similar to Cases 1 and 4, were run, except, the heat flux was reduced by one-half. Refer to Table 5.2.3 to follow the discussion. The effect of reducing the heat load on a 90% full pan with crystals, Case 6, was to reduce recirculation by half as well as the volume averaged variance of the supersaturation in comparison to Case 1. The effect on the CSD would, therefore, be small. However, comparing Case 7 to Case 4, which have no crystals, the reduced heat load in Case 7 caused a 400% reduction in recirculation over Case 4, but, the

reduction in the variance is only by a half, suggesting the effect of the heat load is sensitive to the conditions in the Pan and its effect on the CSD is also. The heat load, besides affecting the fluid dynamics, also affects the batch time needed to produce a desired product. During the course of the batch, the heat load must vary to match the program of evaporation needed to assure that the proper level of supersaturation is maintained for the growth of crystals. This suggests that the real effect, for example, of reduced steam pressure, cannot be evaluated without simulating the entire batch. But the experiment does demonstrate that there is a significant effect of the heat load on the Pan.

Changing the pressure in the Pan vapor space directly effects the boiling temperature in the Pan. Therefore, a Pan operating at an increased pressure, given everything else is equal, one would expect the recirculation to increase as a result of a reduced viscosity of the liquid. However, increasing the average temperature in the Pan also decreases the supersaturation in the Pan and hence, if one desires to maintain the supersaturation at a controlled set point, the brix in the Pan must be increased, which of course, increases the viscosity of the liquid. Therefore, two cases were run at an increased pressure to demonstrate the interaction between a change in supersaturation and a change in pressure. Maintaining

approximately the same supersaturation at a higher pressure, Case 5, the model predicted a higher recirculation but no change in profile. But, the model predicted something surprising for the run at higher pressure but lower supersaturation, Case 11, the recirculation increased as expected but the profile changed completely. This can be seen by comparing Figures 5.3.1 (5) and (11). This unexpected prediction results mainly from the interaction of the effect of temperature and brix on the viscosity of the fluid. At the lower brix the recirculation is fast enough that the fluid passing through the tubes does not boil in the tubes or just outside the tubes, therefore, the fluid simply rises to the surface to boil. But, in the other cases the recirculation is just low enough to cause some vapor to be formed in the tubes or just outside the tubes which in turn causes mixing at the tube exit, which then develops into the profile observed.

The previous cases discussed, Cases 1 thru 11, were all for high purity massecuite and therefore, the conditions and results are exemplary of high purity batch operation. Case 12 is exemplary of a typical low purity run. As can be seen in Table 5.2.3 and Figure 5.2.1 (1) - (12), the profile in the Pan Proper and pan statistics are similar to many others, but the recirculation is much slower. These effects are basically

due to the lower heat load and the increased viscosity of the fluid.

The experiments as a whole, demonstrate that there are significant supersaturation profiles in the Pan as shown by the volume average variance of the supersaturation and the maximum and minimum supersaturation, as shown in Table 5.3.3. Noting the growth profiles for each case, Figures 5.2.2 (1) - (12), one can observe that there are differences in the growth rates throughout the Pan. The differences throughout the Pan will cause a widening of the CSD as the batch proceeds. The extent of the widening of the CSD, as the result of growth variations and nucleation of new crystals, cannot be determined without a population balance in combination with the fluid dynamics. The model demonstrates that there is a large difference between the maximum and minimum supersaturation (growth rates), indicating that if a poor control system is used, excessive nucleation may occur or the average growth rate may be too low. This phenomenon may occur particularly when the level is low because the average Pan temperature is higher at this time resulting from the fact that a larger fraction of the total volume is contained in the tubes and because the heating rate per unit volume is larger. But, even though the Pan average temperature is higher, the temperature at the surface is limited by its boiling

point. Thus, to avoid nucleation at the surface the Pan average growth rate may need to be lower than expectations suggest, based on the average conditions in the Pan. Figures 5.2.2 (1) - (12), of course, demonstrate the existence of the maximum growth rates occurring at the surface and the minimum in the tubes. The model offers an inexpensive method to study the various profiles in the Pan and qualitatively simulate the application of a control system.

Referring again to the velocity profiles, Figures 5.2.1 (1) - (12), and the growth rate profiles, Figures 5.2.2 (1) - (12), one can observe that if the velocity profiles are similar between the cases, the growth rate profiles are similar. This results from the fact that for no spatial differences in concentration in the Pan the growth rate profile is entirely dependent on the temperature profile. But, of course, the temperature profile, because the effect of diffusion is small, is greatly dependent on convection. This reinforces the importance of good circulation in the Pan. The more turbulence that is generated in the Pan Proper, the more uniform the growth profile. This point is typified in Figure 5.2.1 (1) and Figure 5.2.2 (1).. However, when the velocity profile is more streamlined (i.e., less turbulent), as in Figure 5.2.1 (11), the growth rate profiles, as in Figure 5.2.2 (11), are

less uniform in the Pan Proper.

TABLE 5.2.1: TYPICAL PAN DESIGNS

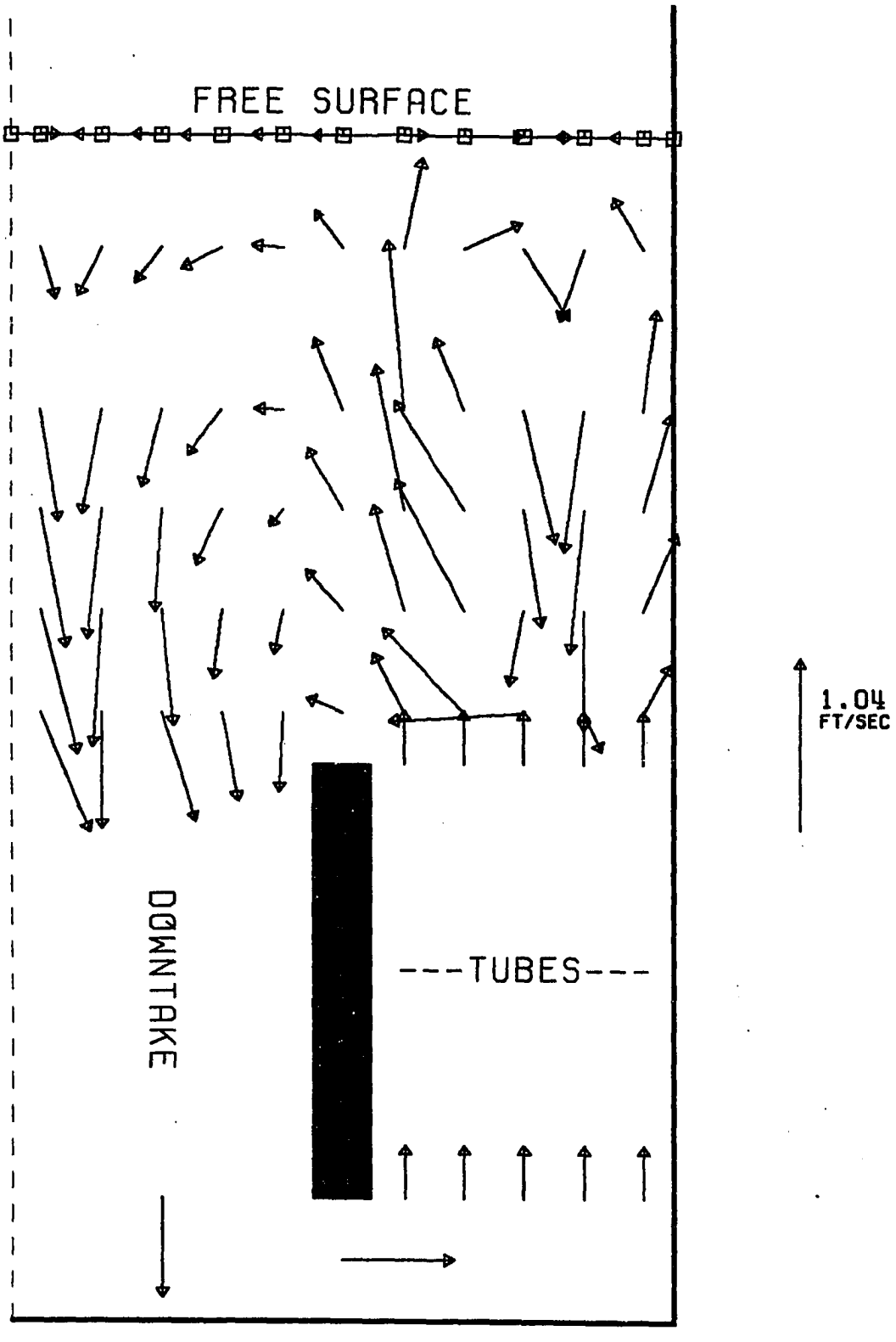
PAN	WVOL (FT^3)	HMAX (FT)	Dp (FT)	Dc (FT)	Dd/Dc %	AREAT/WVOL	TUBES NTUBES	TUBES TUBED (IN)	TUBES TUBEH (FT)
A	1200	12.1	12	12	45.5	1.5	343	5	4
B	1200	12.4	12	12	36.4	1.5	343	5	4
C	955	10.0	12	10.9	40.0	1.5	455	4	3
D	1200	12.2	12	12	50.0	1.4	356	4.5	4

TABLE 5.2.2: LOG OF MODEL RUNS VARYING PAN DESIGN AND OPERATING CONDITIONS

CASE	PAN	BRIX	PURITY	HEAT RATE $(\frac{BTU}{HR})$ x10^7	P (PSIA)	CRYSTALS γ_c	CRYSTALS L $(FT)_4$ x10^4	LEVEL % MAX	LEVEL ABOVE CALANDRIA (FT)
1	A	.800	.94	2.69	2.00	.181	3.28	90	5.79
2	A	.800	.94	2.69	2.00	.181	3.28	75	3.98
3	B	.800	.94	2.69	2.00	.181	3.28	90	5.79
4	A	.800	.90	2.69	2.00	0	0	90	5.79
5	A	.824	.94	2.69	3.72	.181	3.28	90	5.79
6	A	.800	.94	1.35	2.00	.181	3.28	90	5.79
7	A	.800	.90	1.35	2.00	0	0	90	5.79
8	C	.800	.94	2.14	2.00	.181	3.28	90	5.00
9	C	.800	.94	2.14	2.00	.181	3.28	81	4.10
10	D	.800	.94	2.51	2.00	.181	3.28	90	5.79
11	A	.800	.94	2.69	3.72	.181	3.28	90	5.79
12	A	.824	.70	.553	2.00	.183	3.28	90	5.79

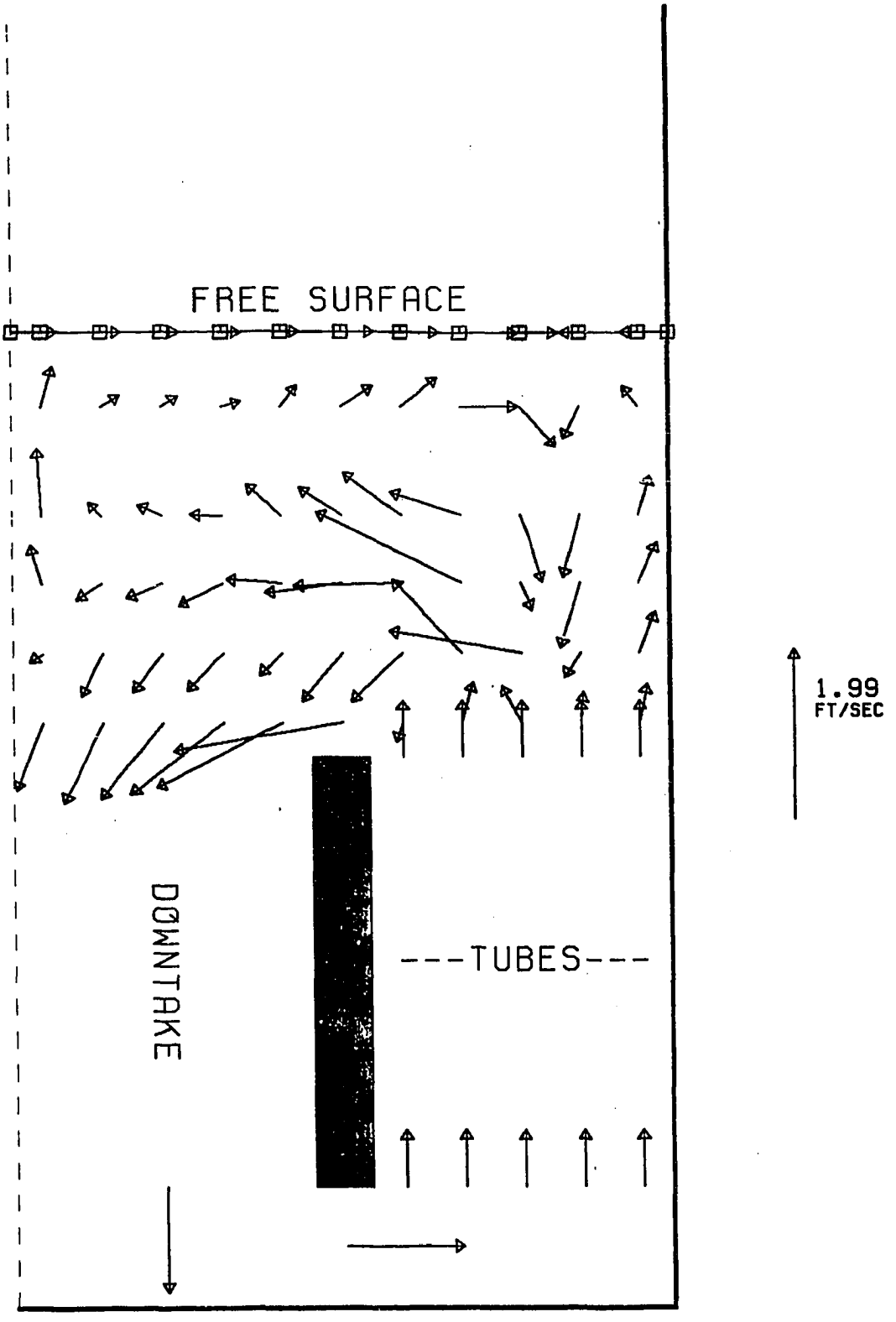
TABLE 5.2.3: SUMMARY OF MODEL RESULTS

CASE	PAN	SUPERSATURATION VOL. AV.	SUPERSATURATION VOL. AV. σ^2 $\times 10^{-3}$	SUPERSATURATION MAX.	SUPERSATURATION MIN.	VOL. AV. ρ $(\frac{LB}{FT^3})$	VOL. AV. T (F)	RECIR. RATE $(\frac{LB}{HR})$ $\times 10^6$	AV. VEL. TUBES $(\frac{FT}{SEC})$
1	A	1.300	1.13	1.339	1.241	89.83	139.6	4.47	.298
2	A	1.284	1.18	1.339	1.231	89.79	141.6	9.21	.612
3	B	1.299	1.20	1.339	1.237	89.83	139.7	4.18	.278
4	A	1.305	.522	1.339	1.269	87.79	138.9	13.3	.976
5	A	1.283	1.51	1.330	1.219	90.12	165.4	5.05	.335
6	A	1.311	.651	1.339	1.264	89.86	138.3	2.95	.196
7	A	1.315	.372	1.339	1.283	87.82	137.8	4.21	.286
8	C	1.301	1.37	1.339	1.220	89.83	139.5	2.91	.229
9	C	1.279	2.36	1.339	1.184	89.78	142.1	3.05	.240
10	D	1.297	1.27	1.339	1.226	89.82	140.0	3.60	.286
11	A	1.094	1.29	1.141	1.032	89.32	164.8	6.12	.409
12	A	1.310	.300	1.326	1.275	90.67	138.5	1.47	.097

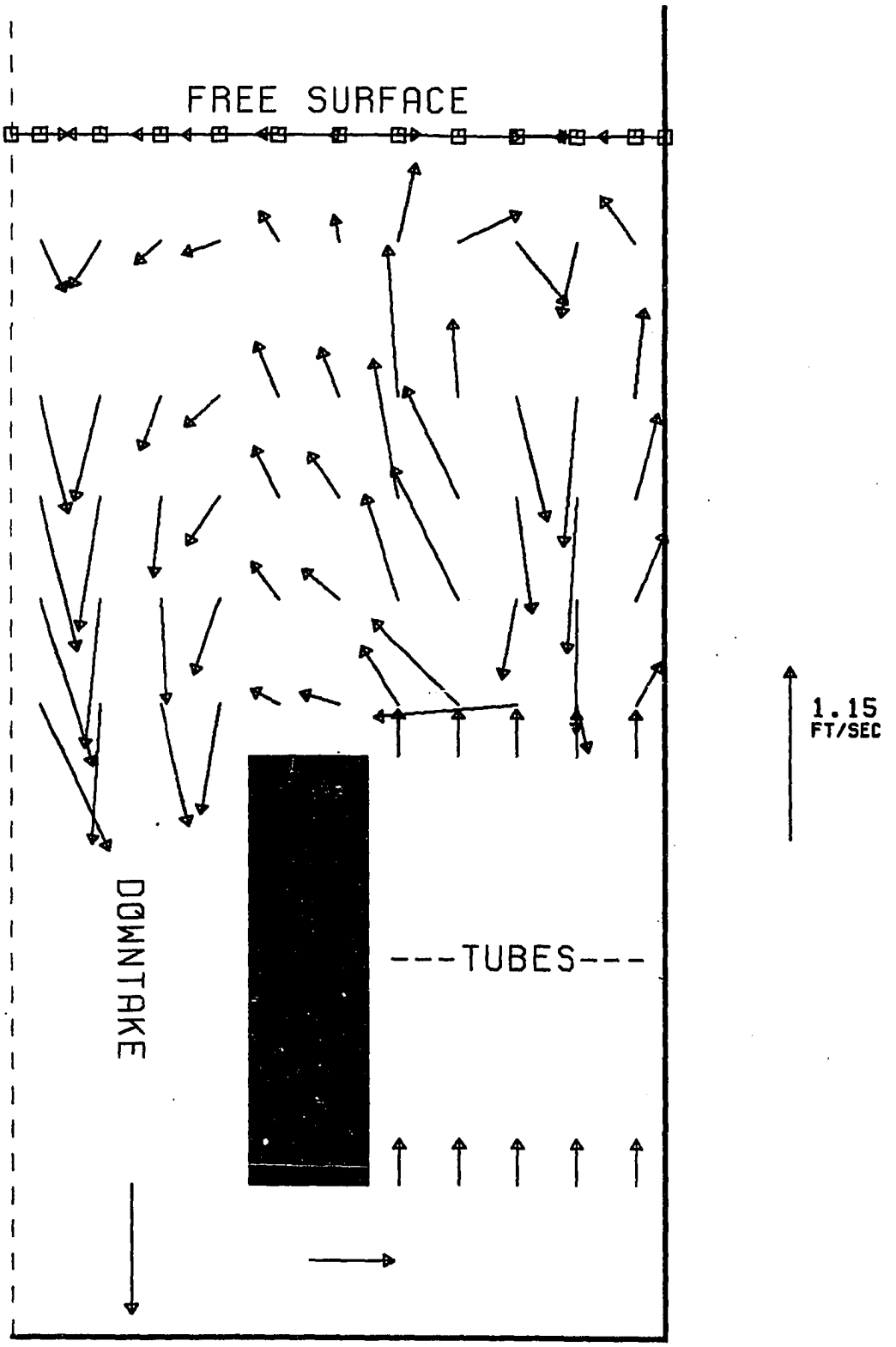


VELOCITY VECTORS FIGURE 5.2.1 (1)

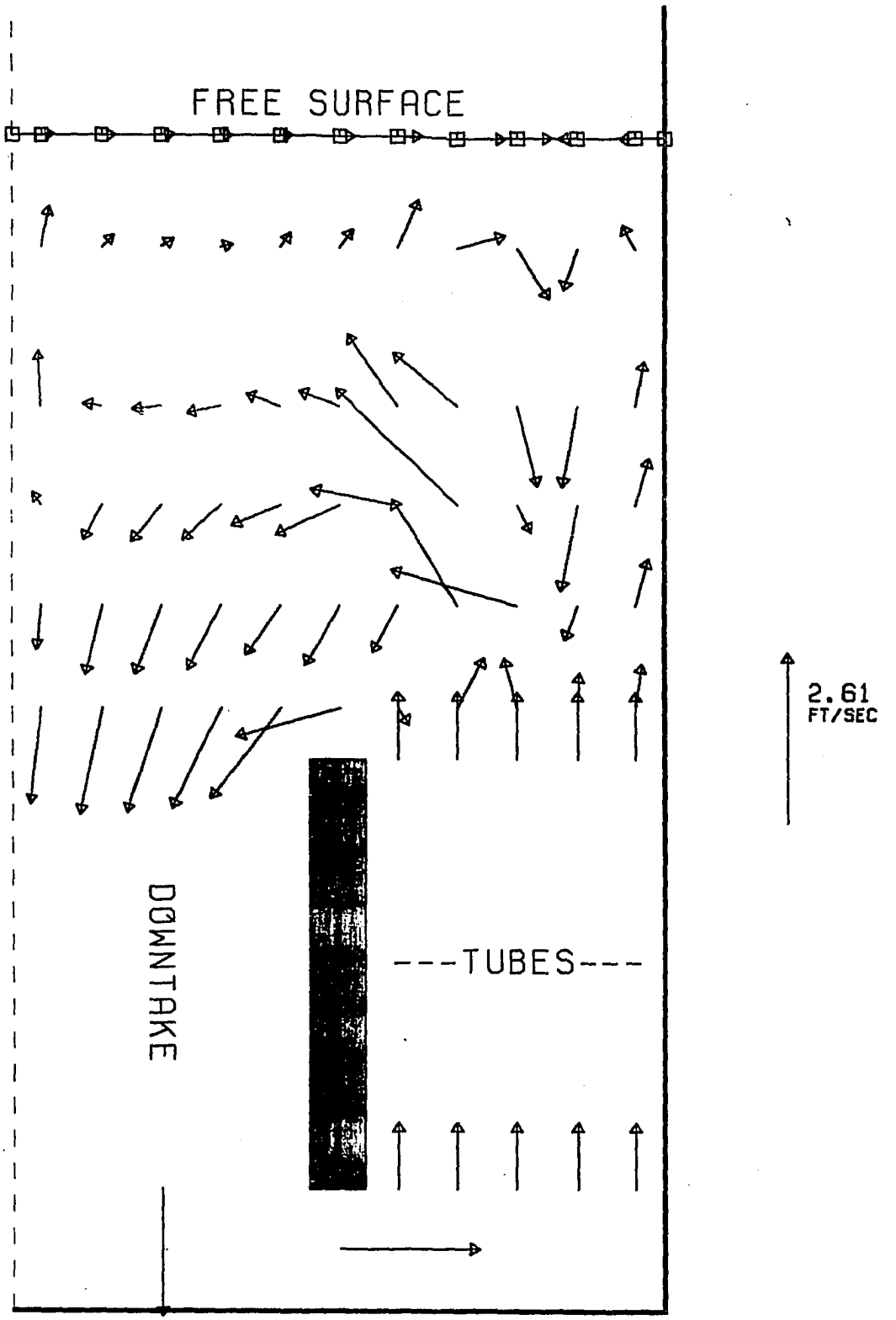
Base Case For Study



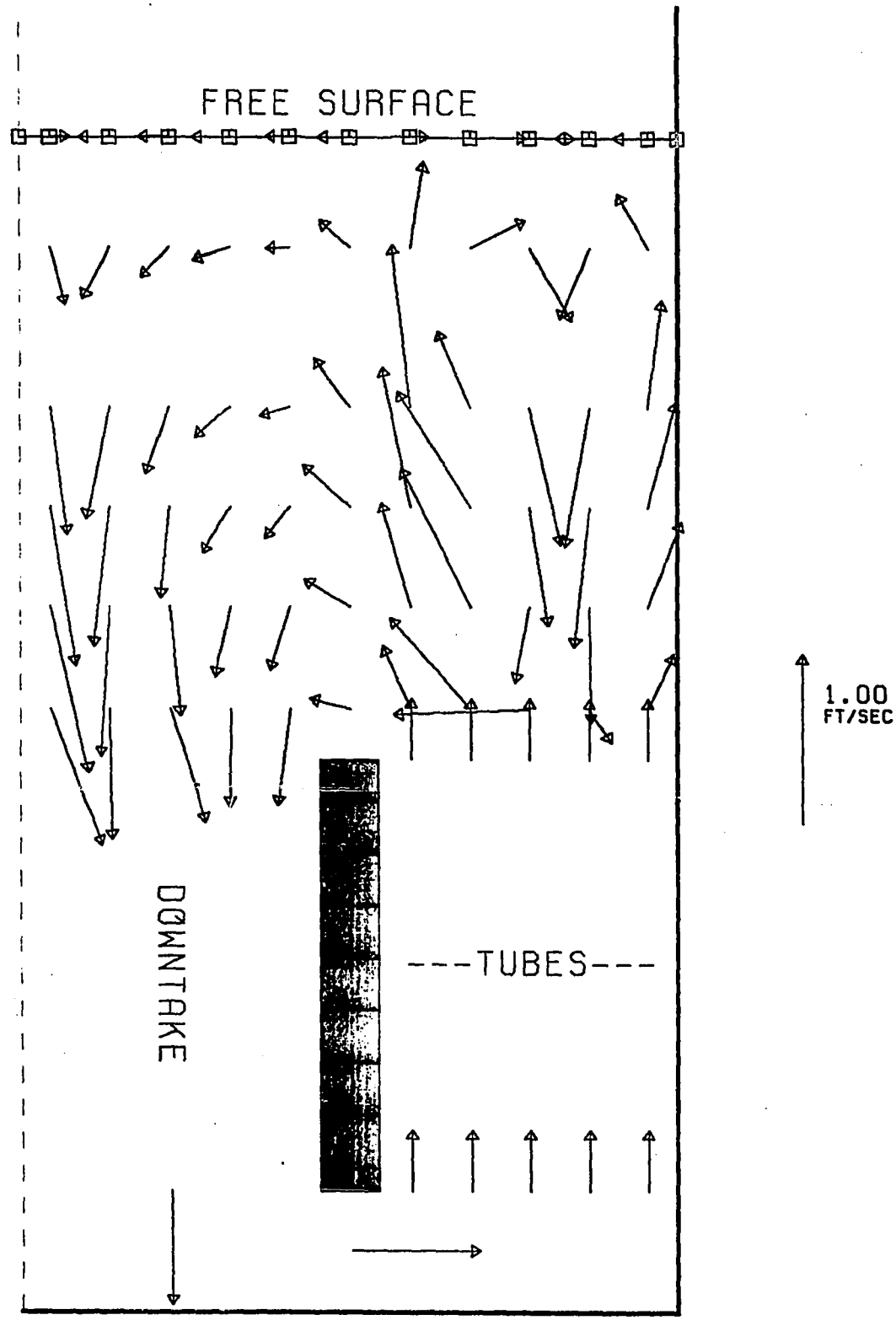
VELOCITY VECTORS FIGURE 5.2.1 (2)
Effect of Reduced Level



VELOCITY VECTORS FIGURE 5.2.1 (3)
Effect of Reduced Downtake Diameter

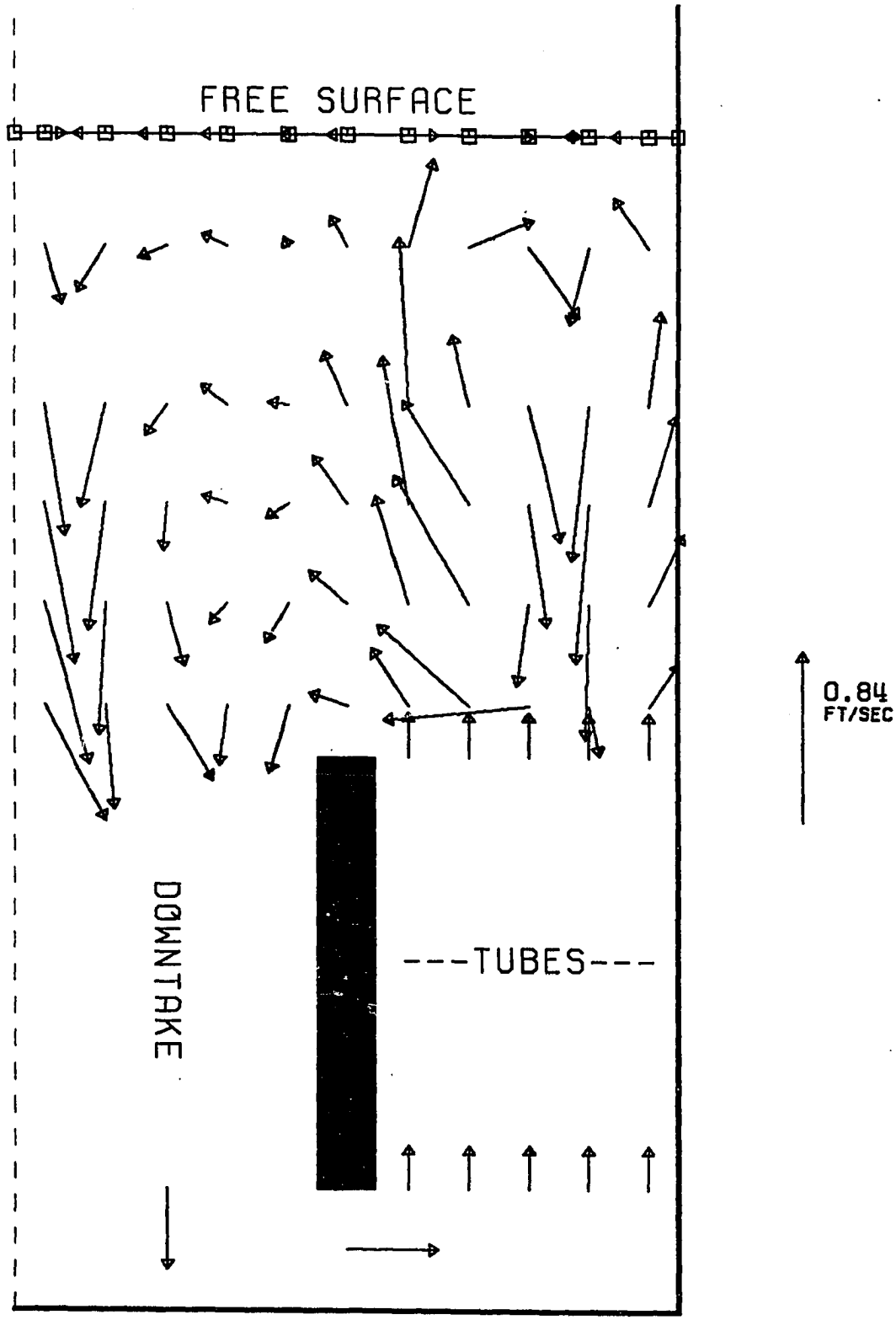


VELOCITY VECTORS FIGURE 5.2.1 (4)
Effect of Reduced Volume Fraction Crystals



VELOCITY VECTORS FIGURE 5.2.1 (5)

Effect of Increased Pressure and Increased Brix



VELOCITY VECTORS FIGURE 5.2.1 (6)
Effect of Reduced Heat Input

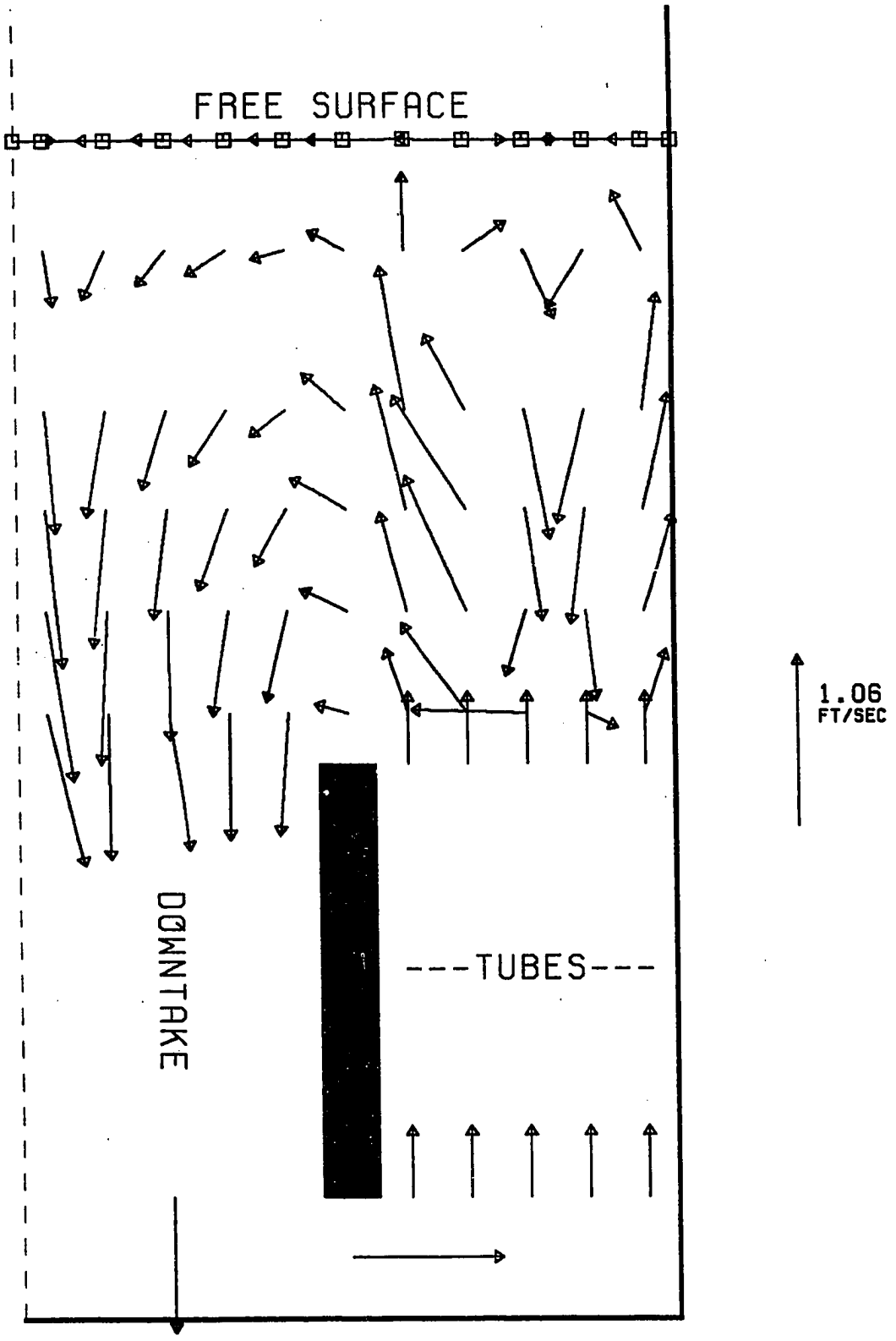
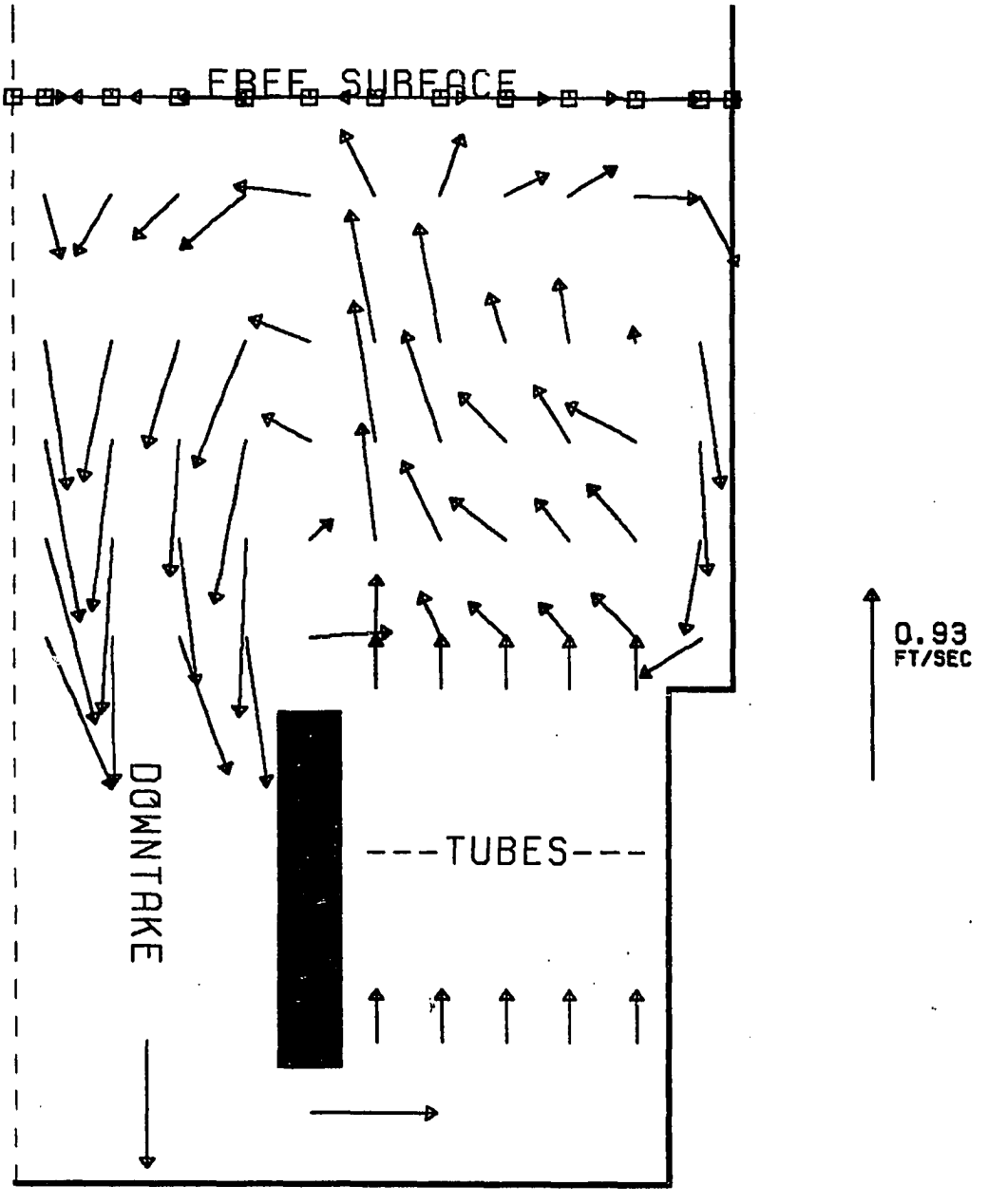
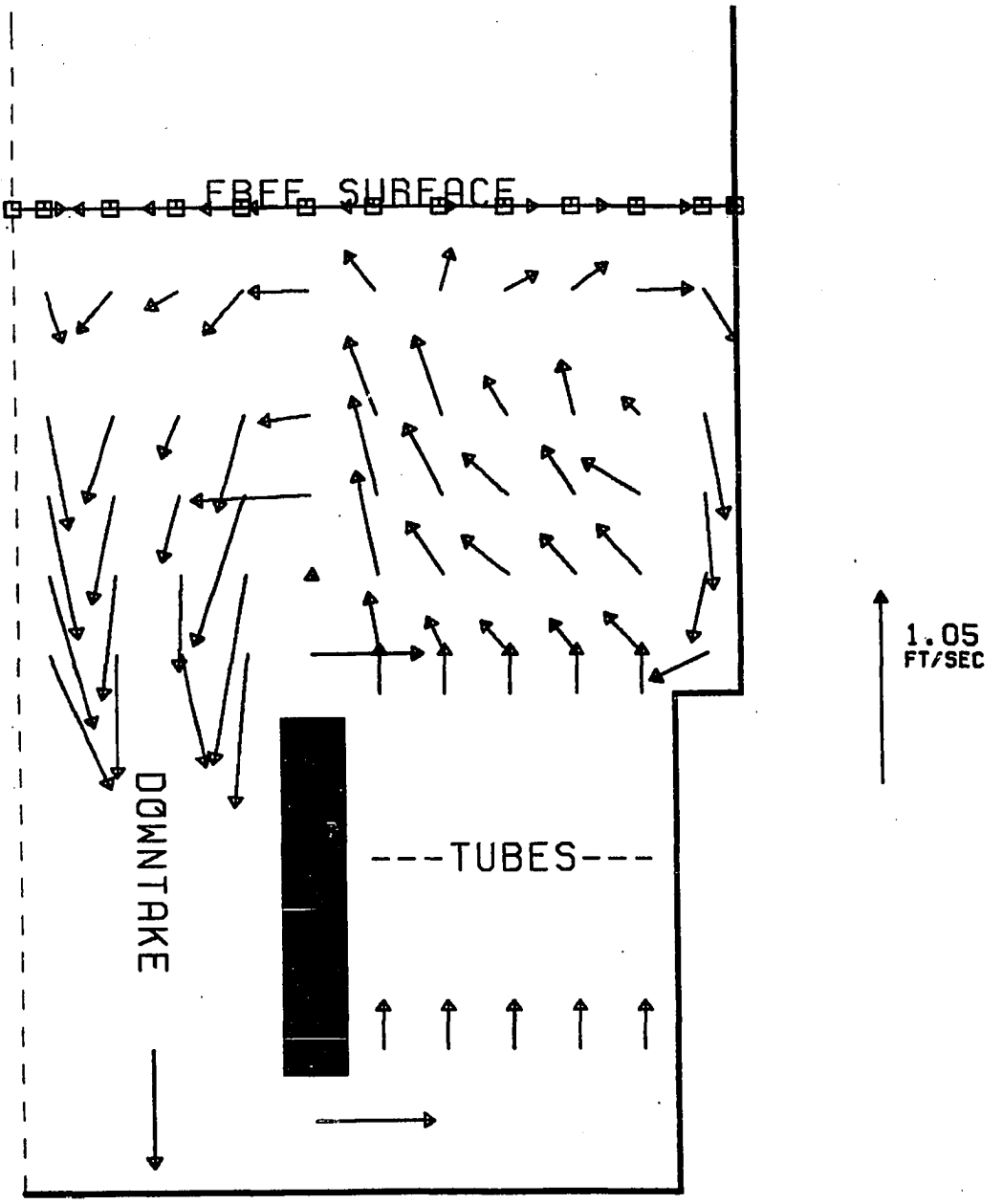


FIGURE 5.2.1 (7)

Effect of Reduced Heat Input and Reduced Volume Fraction Crystals

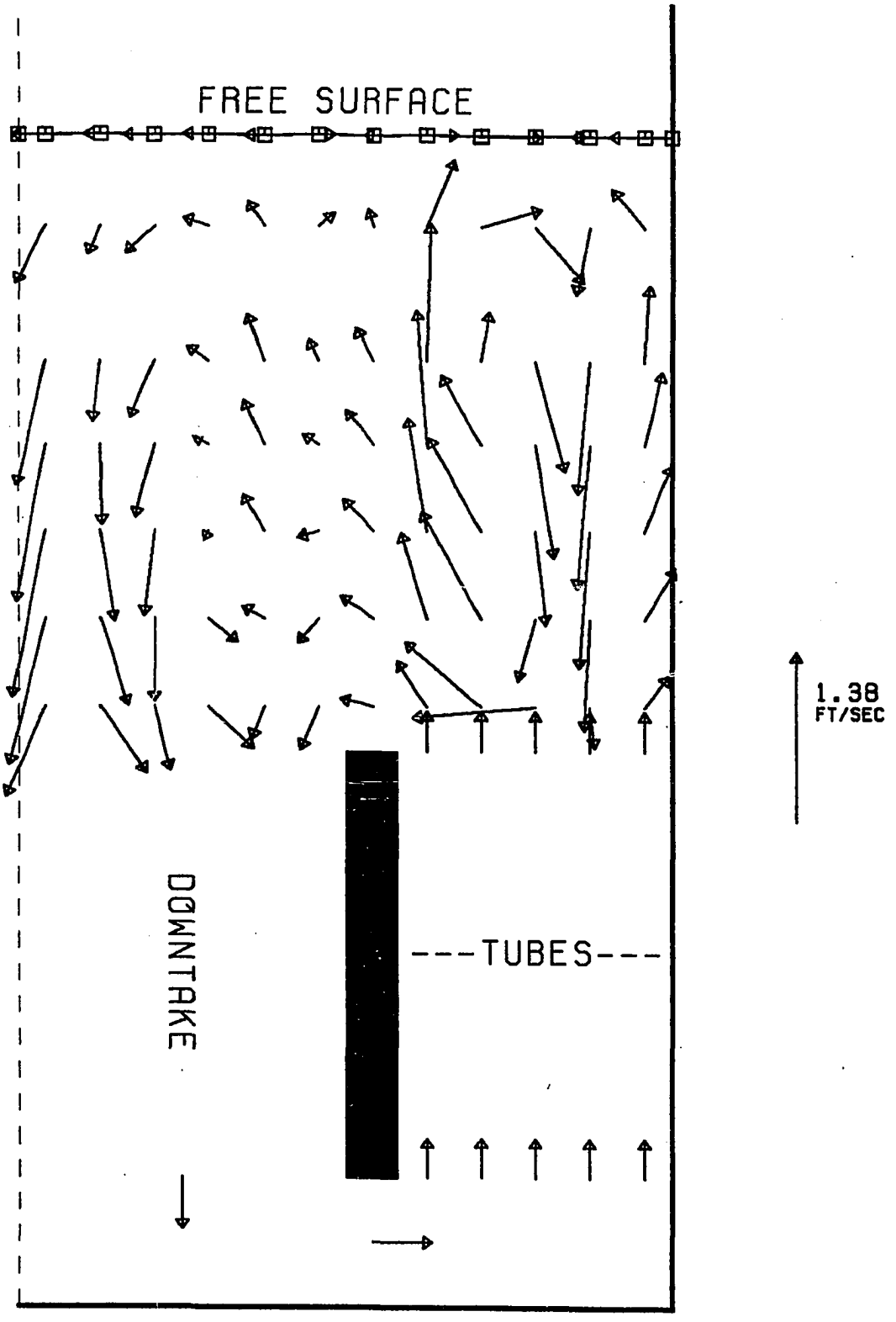


VELOCITY VECTORS FIGURE 5.2.1 (8)
Effect of Increased Major Pan Diameter

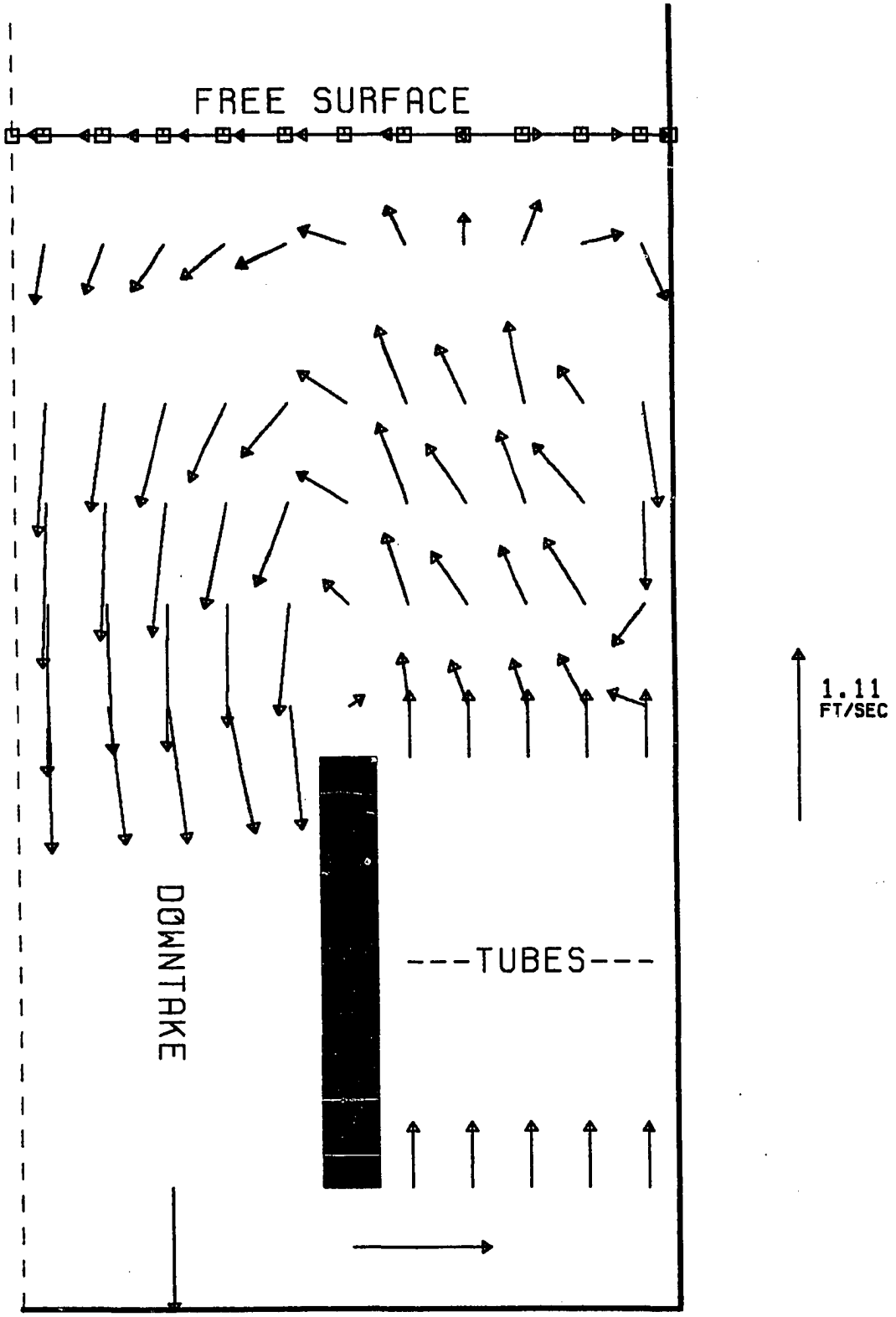


VELOCITY VECTORS FIGURE 5.2.1 (9)

Effect of Increased Major Pan Diameter and Reduced Level

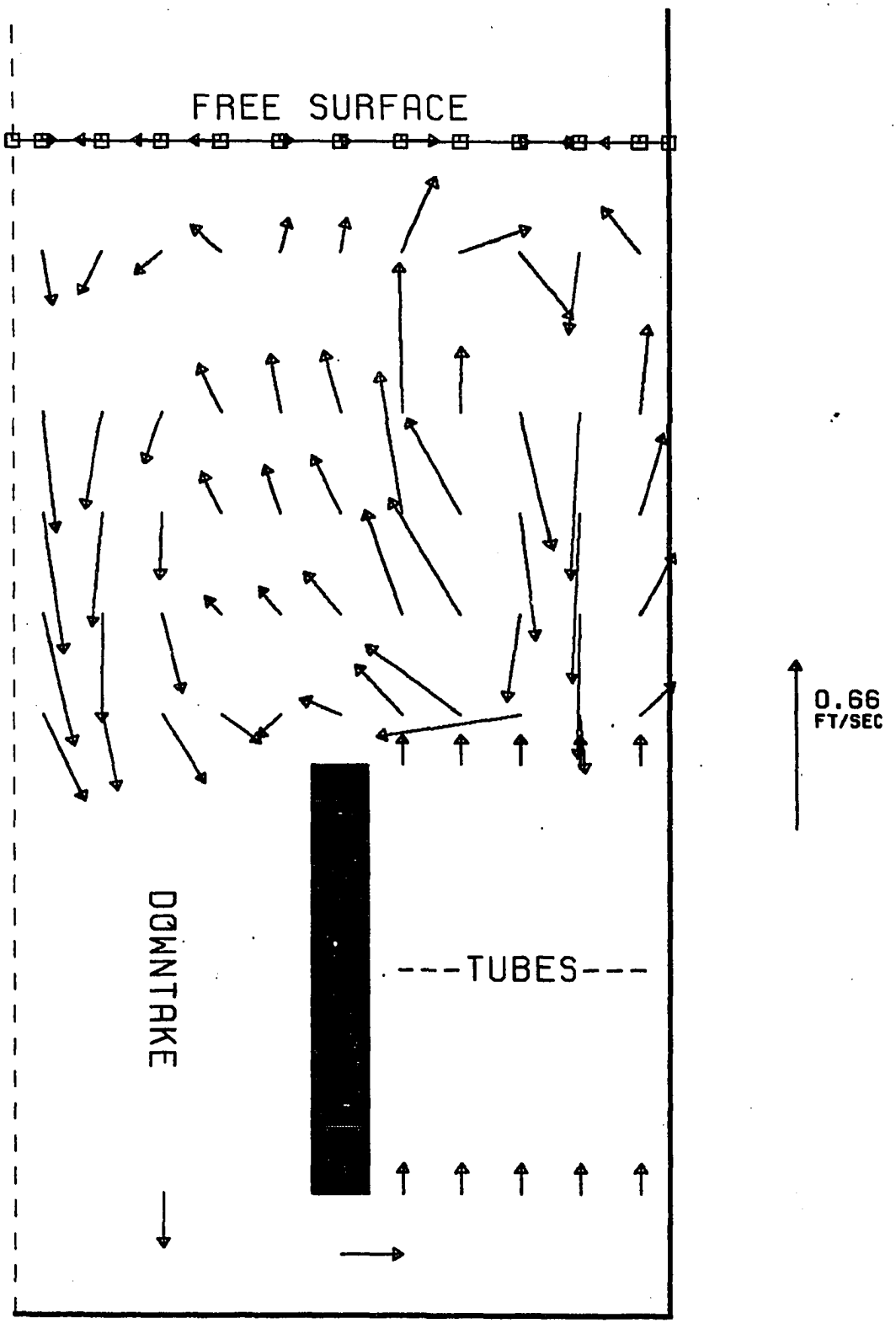


VELOCITY VECTORS FIGURE 5.2.1 (10)
Effect of Increased Downtake Diameter

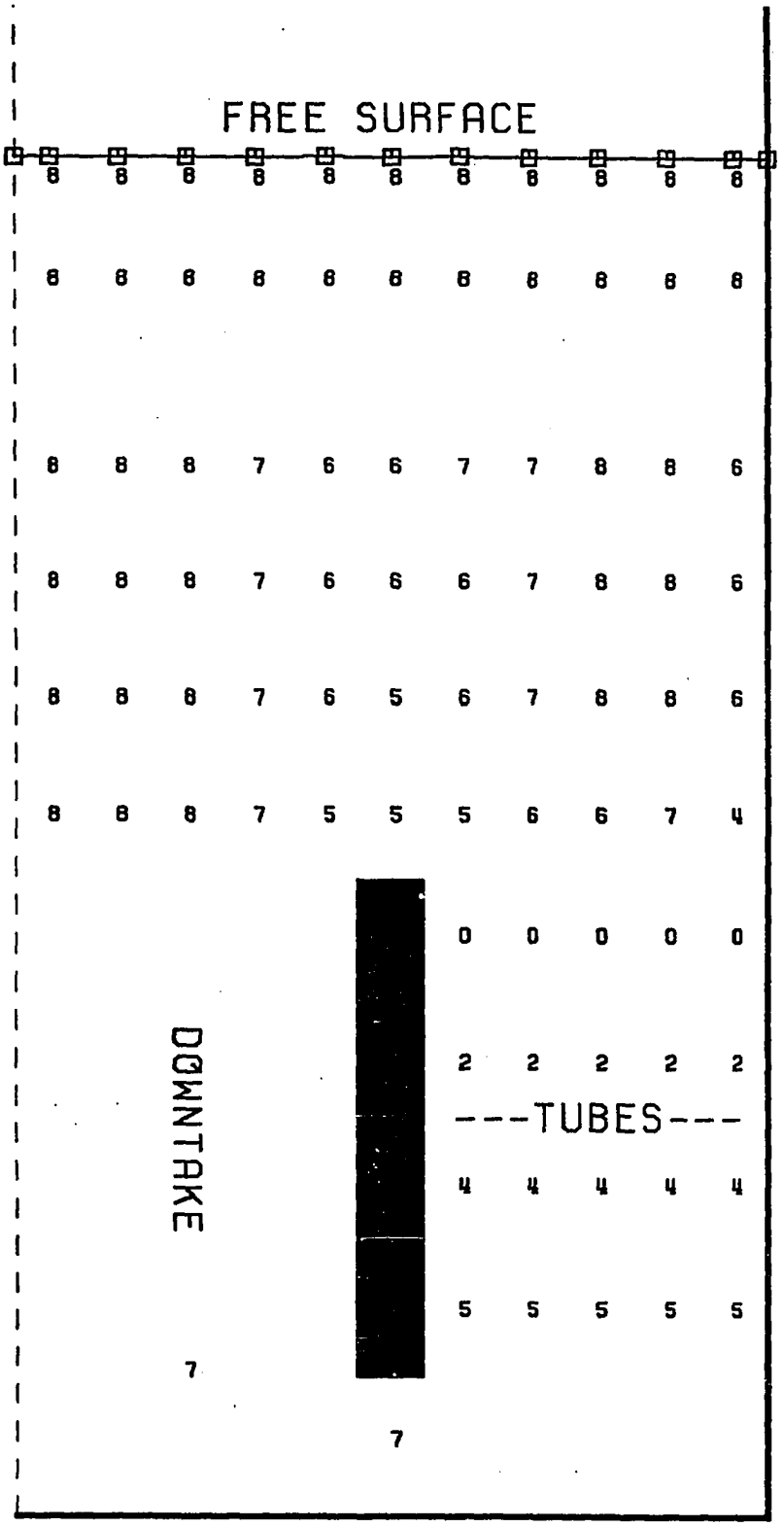


VELOCITY VECTORS FIGURE 5.2.1 (11)

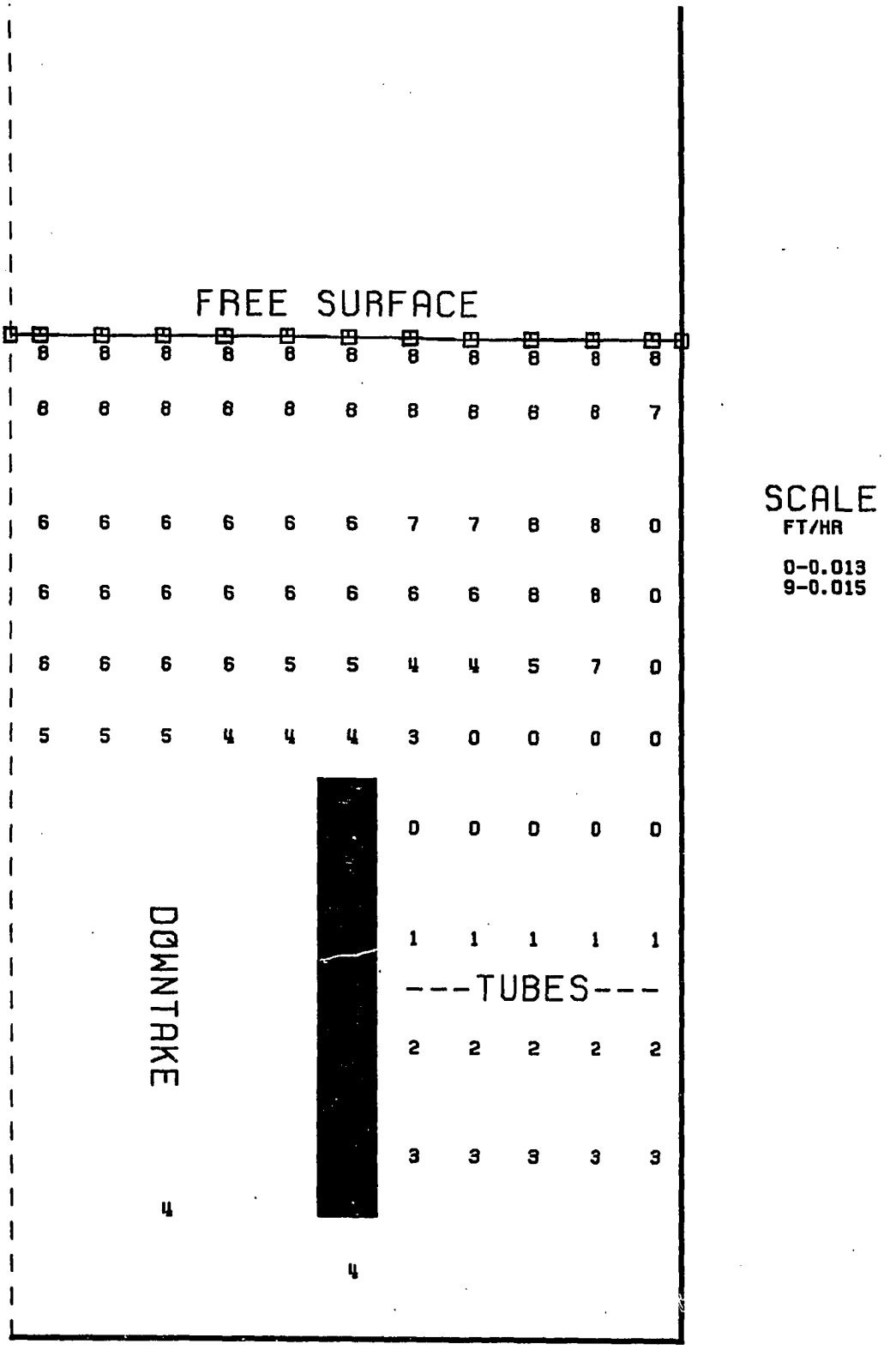
Effect of Increased Pressure and Reduced Supersaturation



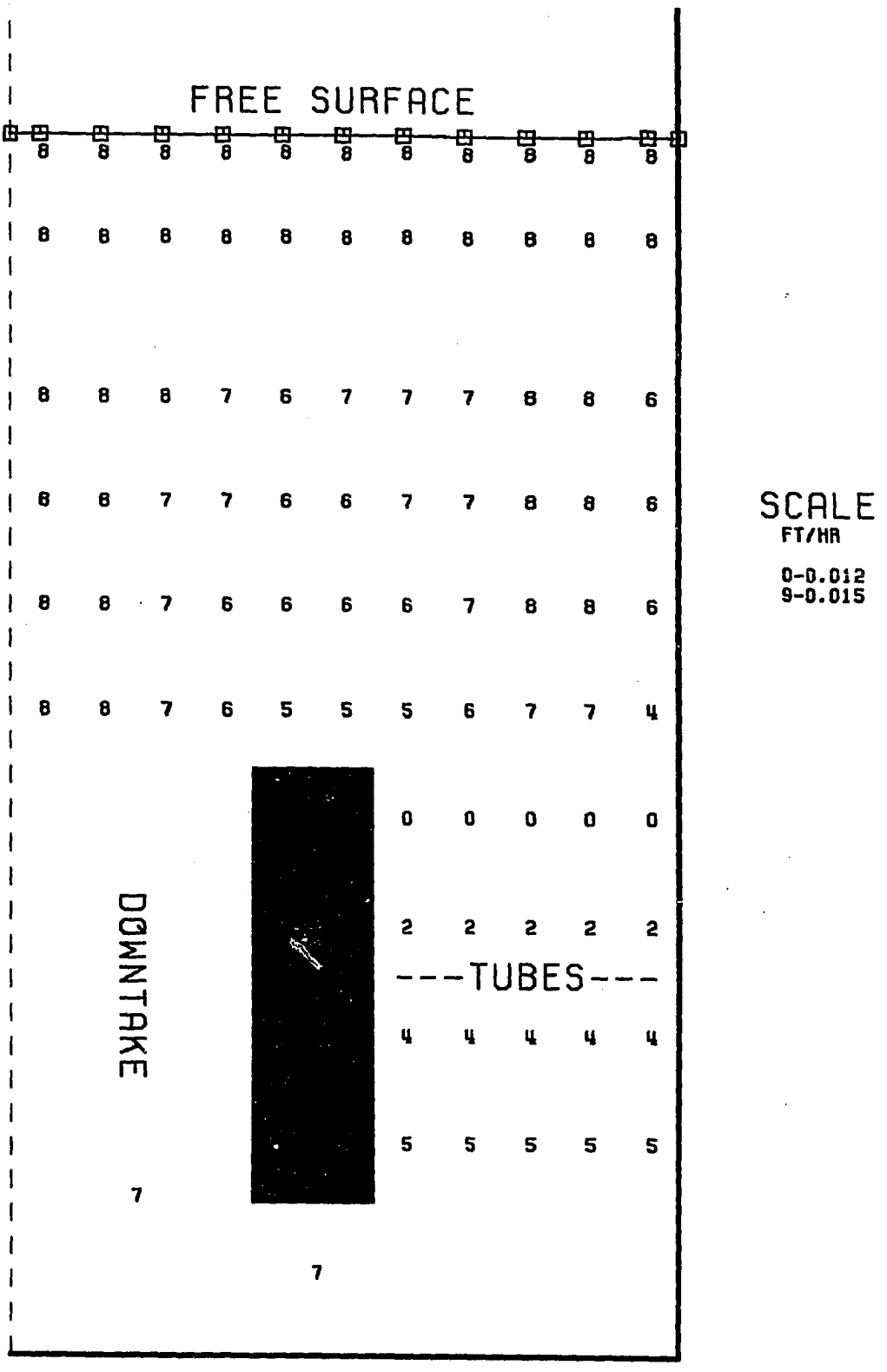
VELOCITY VECTORS FIGURE 5.2.1 (12)
Effect of Low Purity



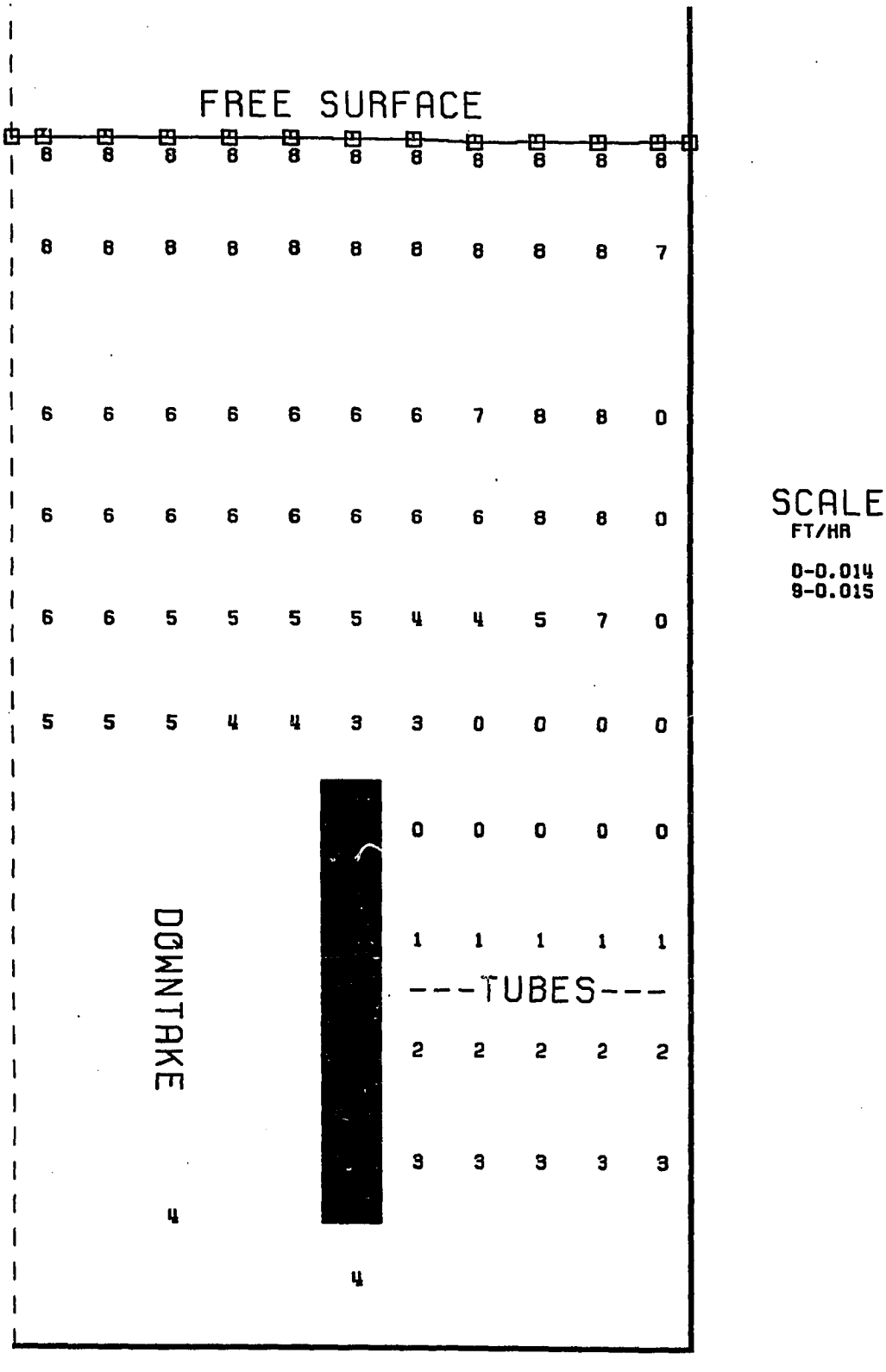
GROWTH PROFILE FIGURE 5.2.2 (1)
Base Case For Study



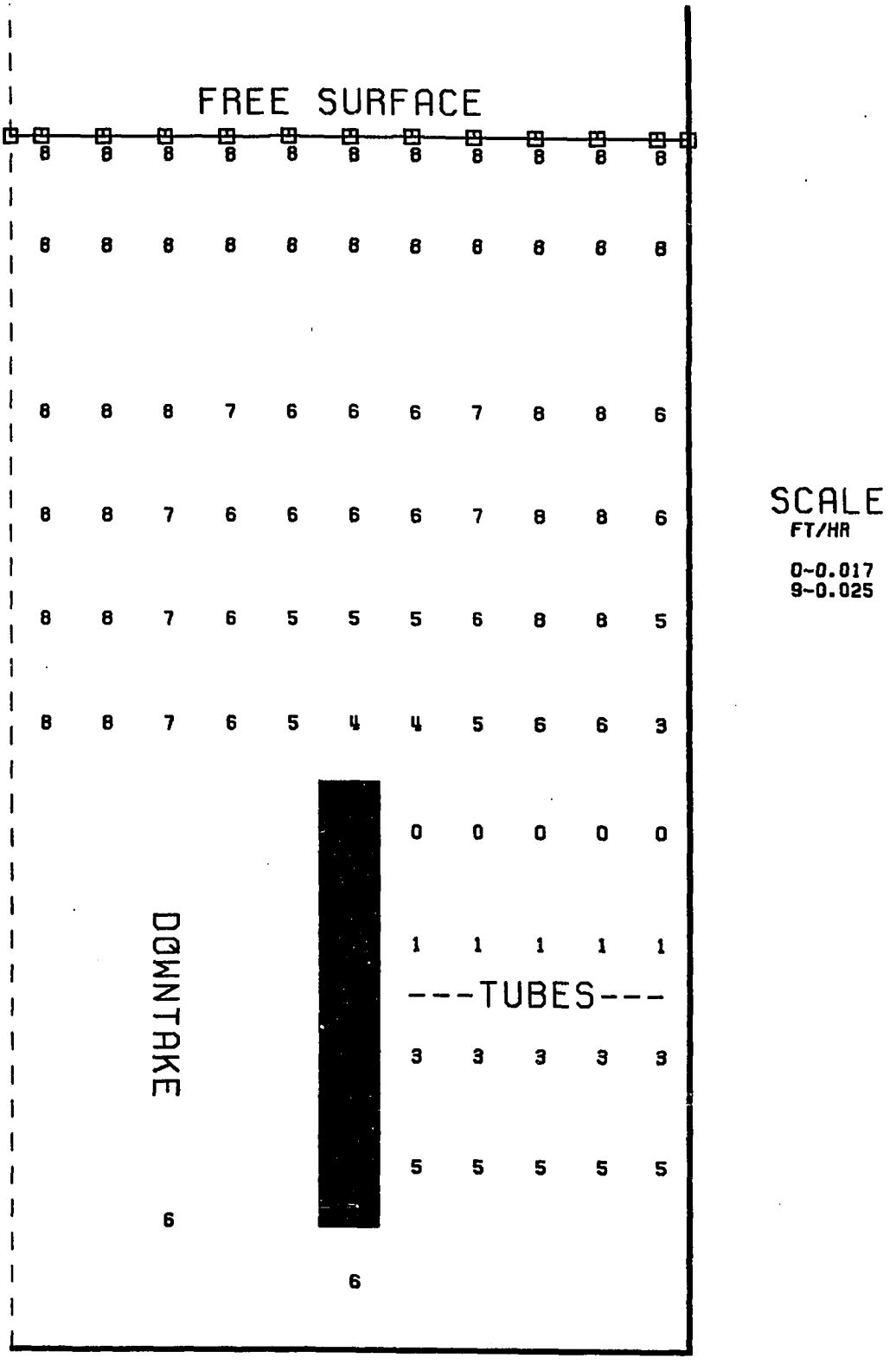
GROWTH PROFILE FIGURE 5.2.2 (2)
Effect of Reduced Level



GROWTH PROFILE FIGURE 5.2.2 (3)
Effect of Reduced Downtake Diameter

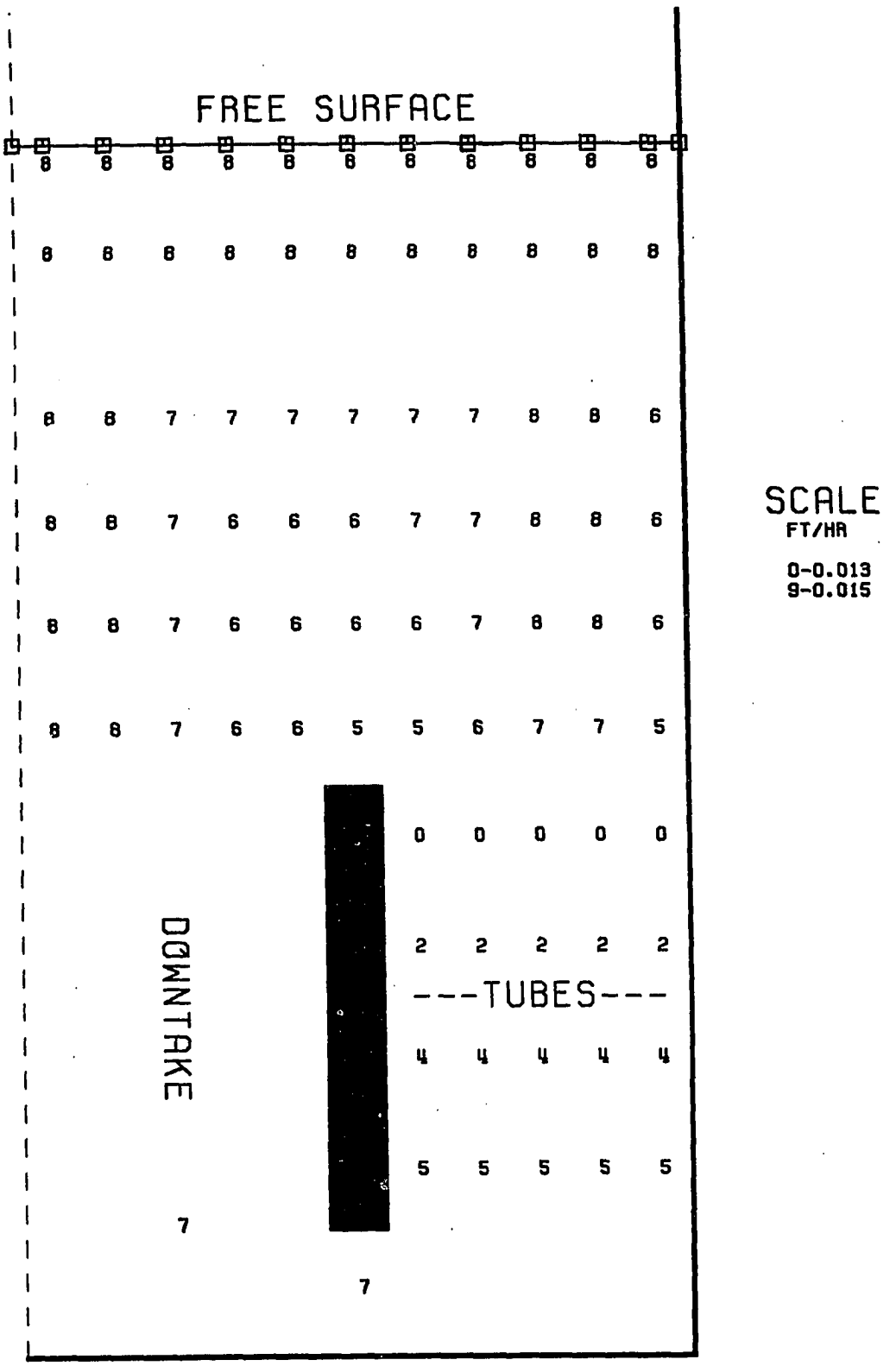


GROWTH PROFILE FIGURE 5.2.2 (4)
Effect of Reduced Volume Fraction Crystals



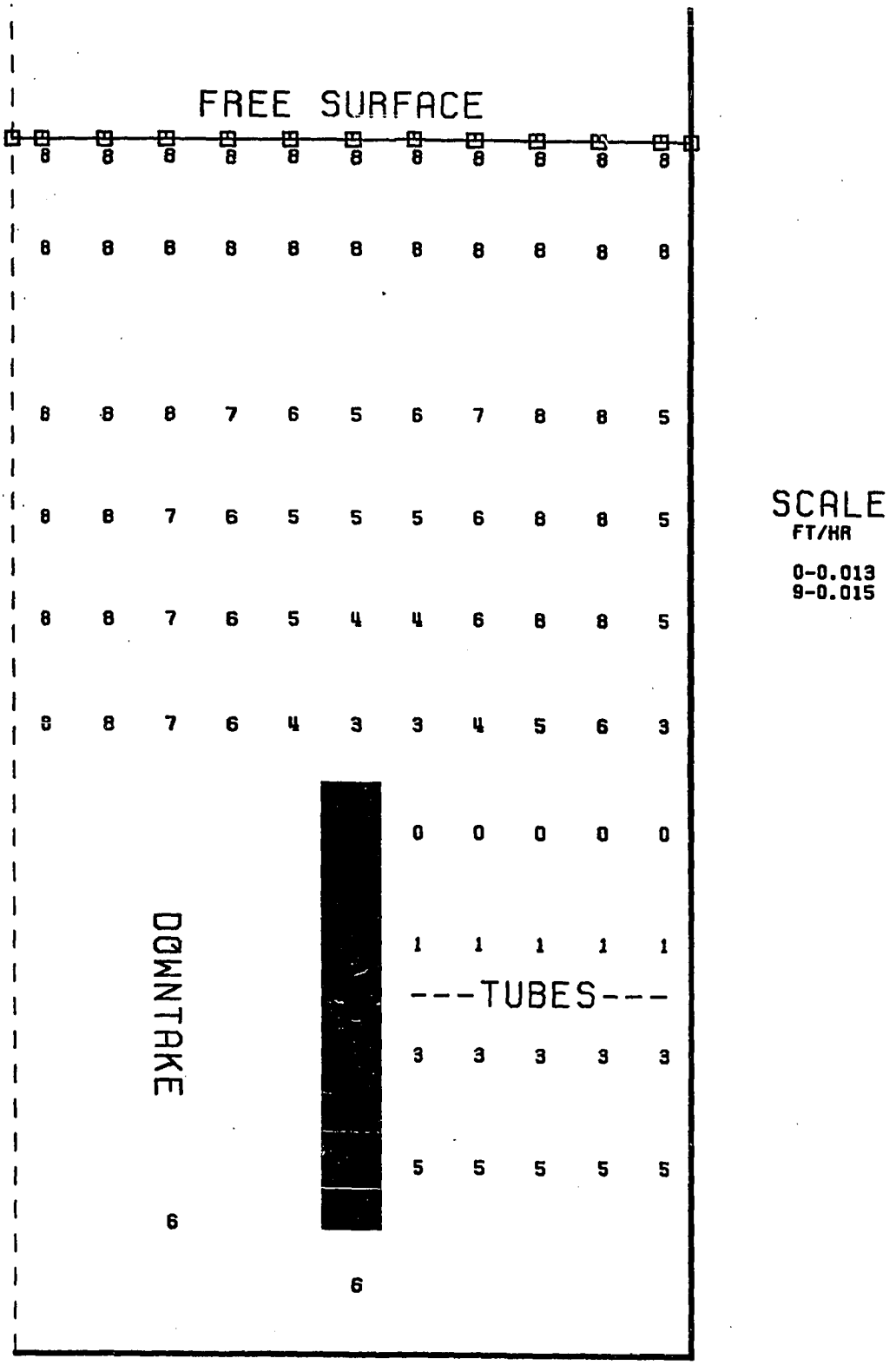
GROWTH PROFILE FIGURE 5.2.2 (5)

Effect of Increased Pressure and Increased Brix



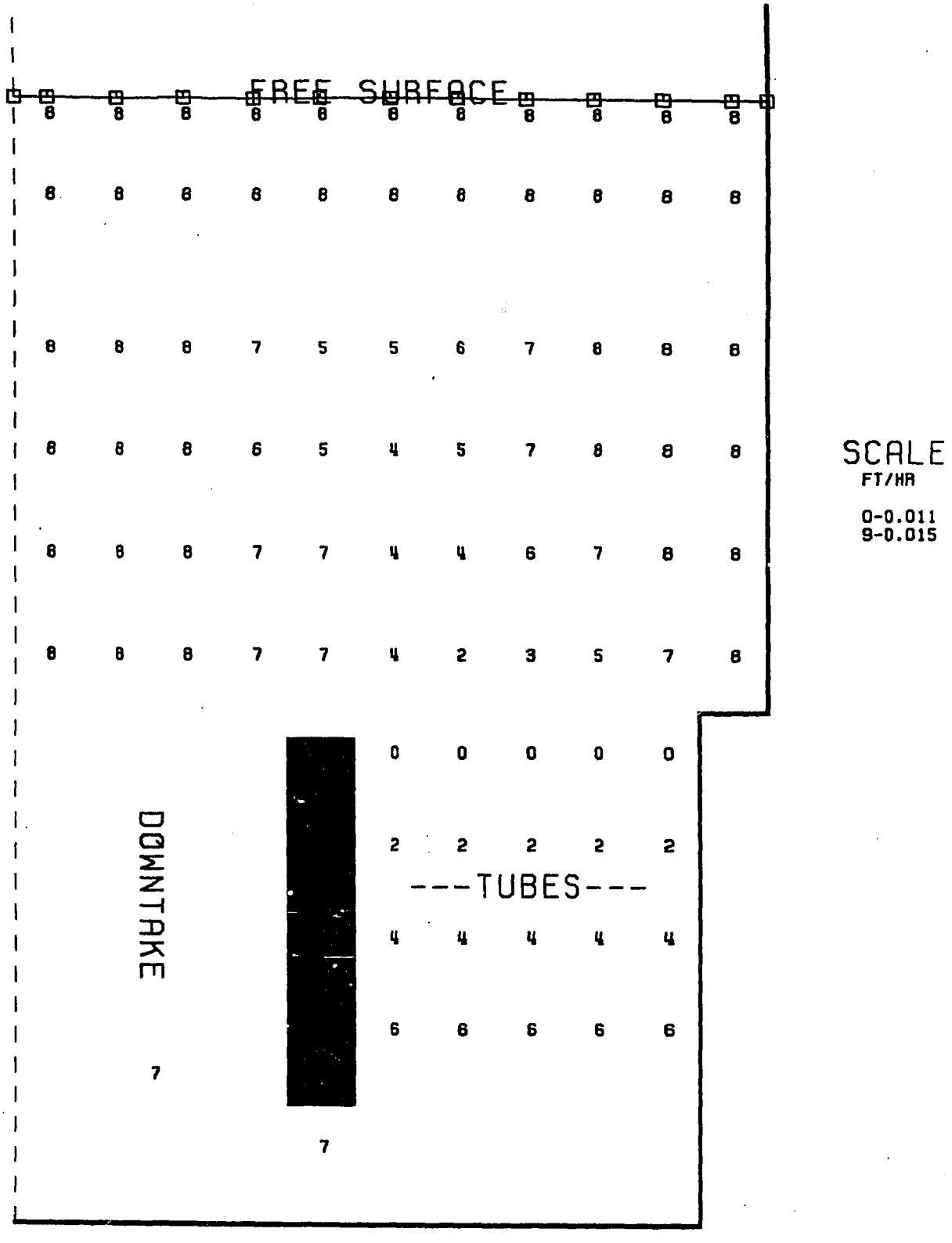
GROWTH PROFILE FIGURE 5.2.2 (6)

Effect of Reduced Heat Input



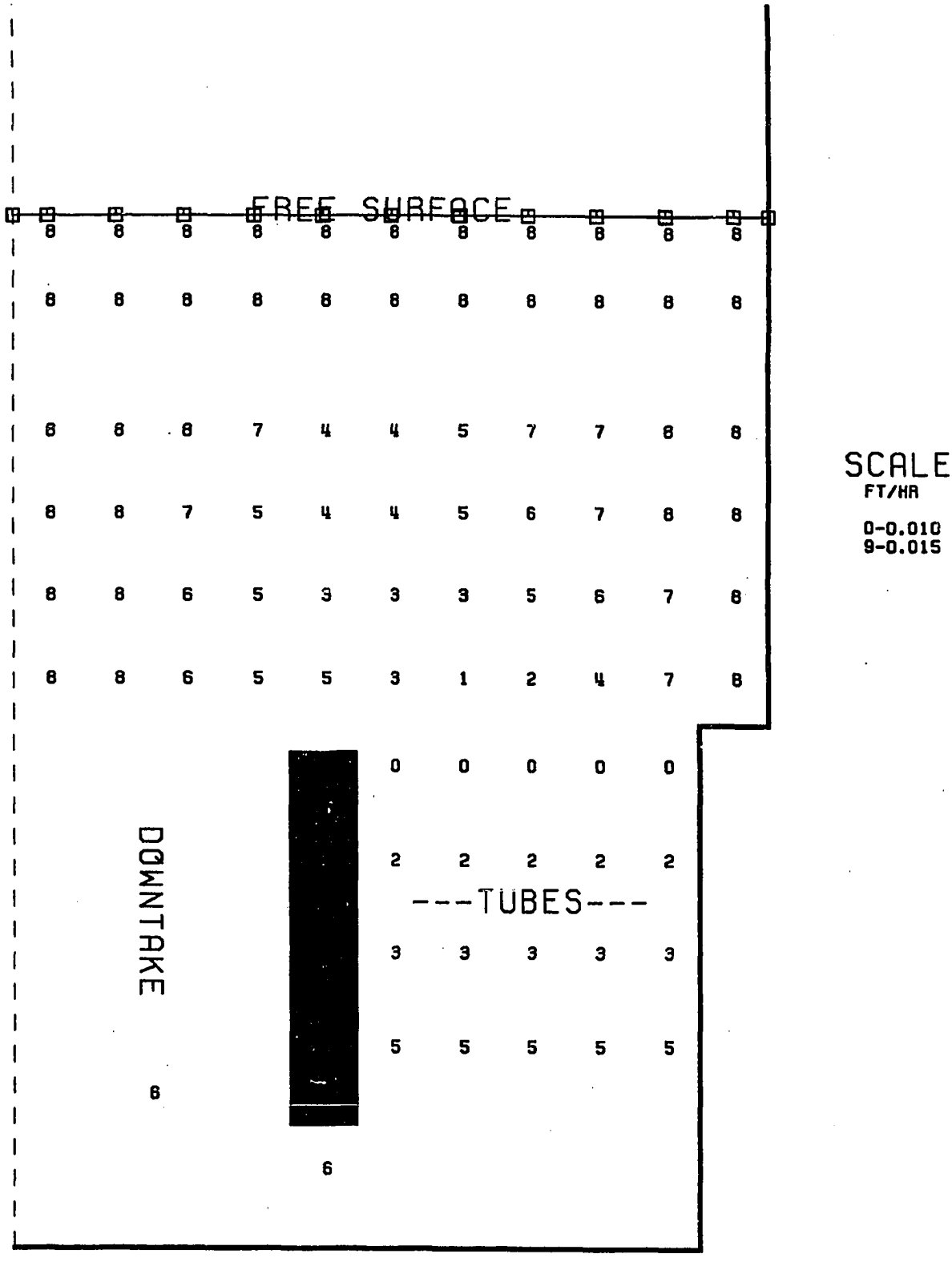
GROWTH PROFILE FIGURE 5.2.2 (7)

Effect of Reduced Heat Input and Reduced Volume Fraction Crystals



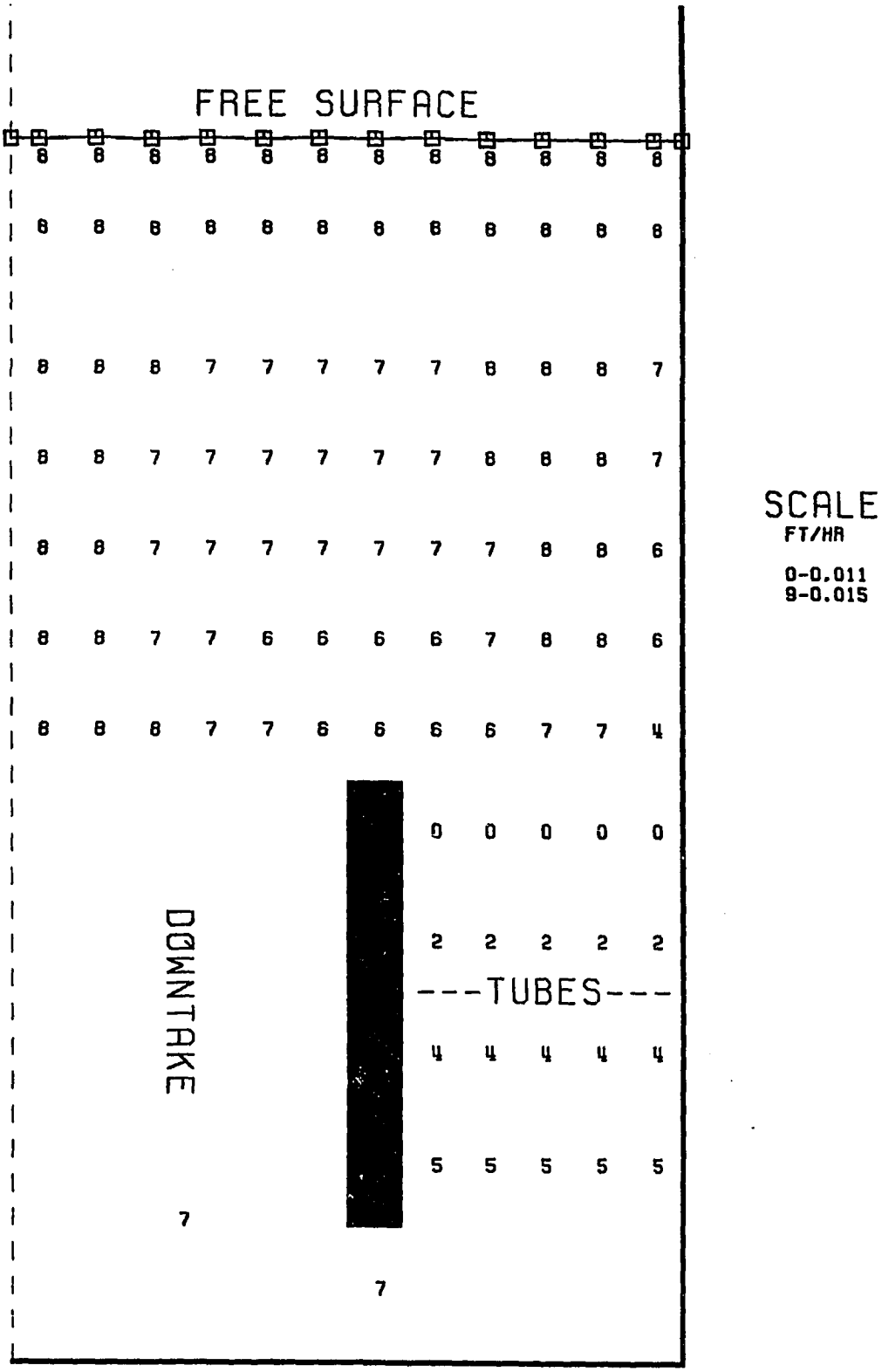
GROWTH PROFILE FIGURE 5.2.2 (8)

Effect of Increased Major Pan Diameter

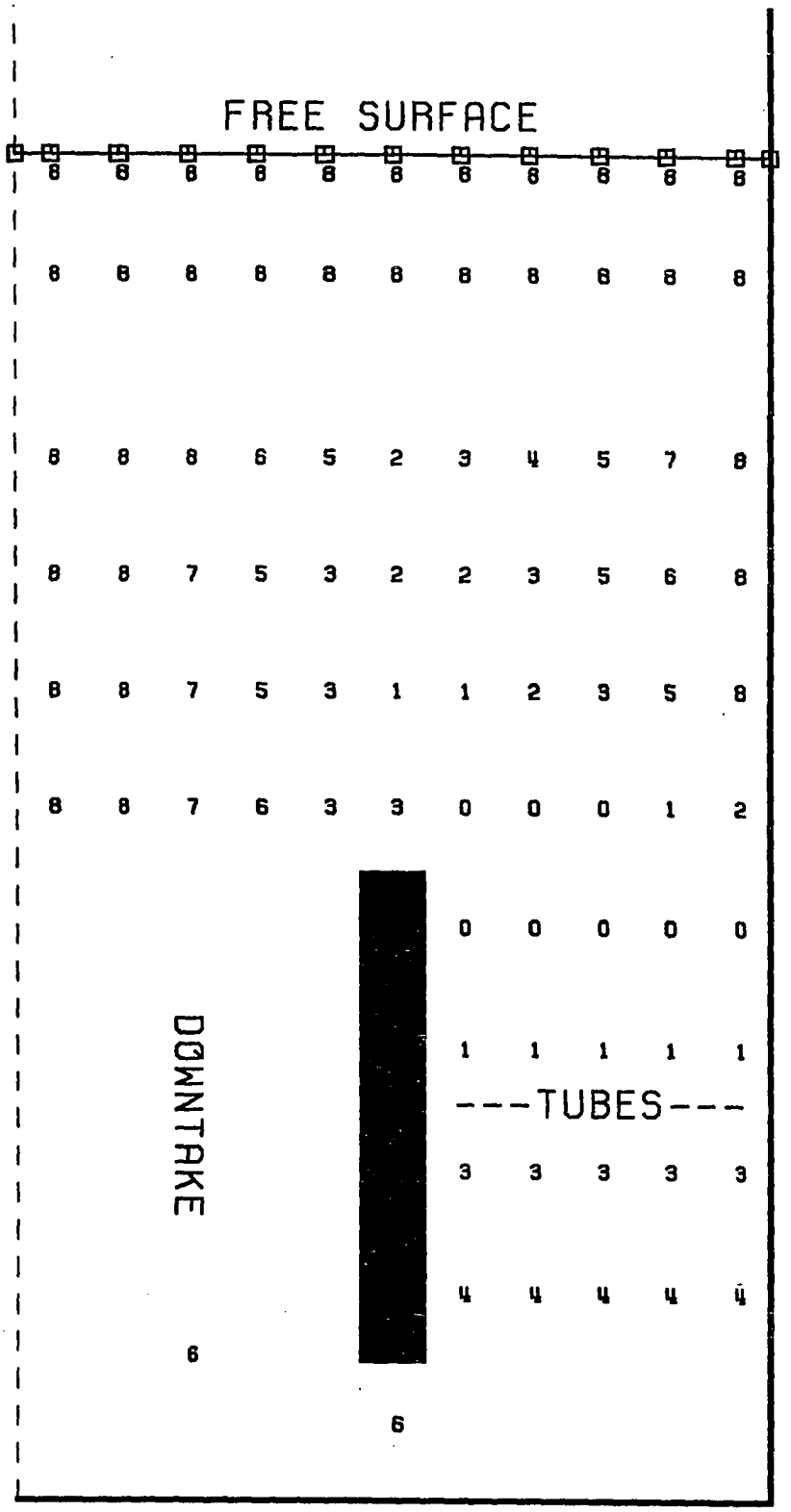


GROWTH PROFILE FIGURE 5.2.2 (9)

Effect of Increased Major Pan Diameter and Reduced Level

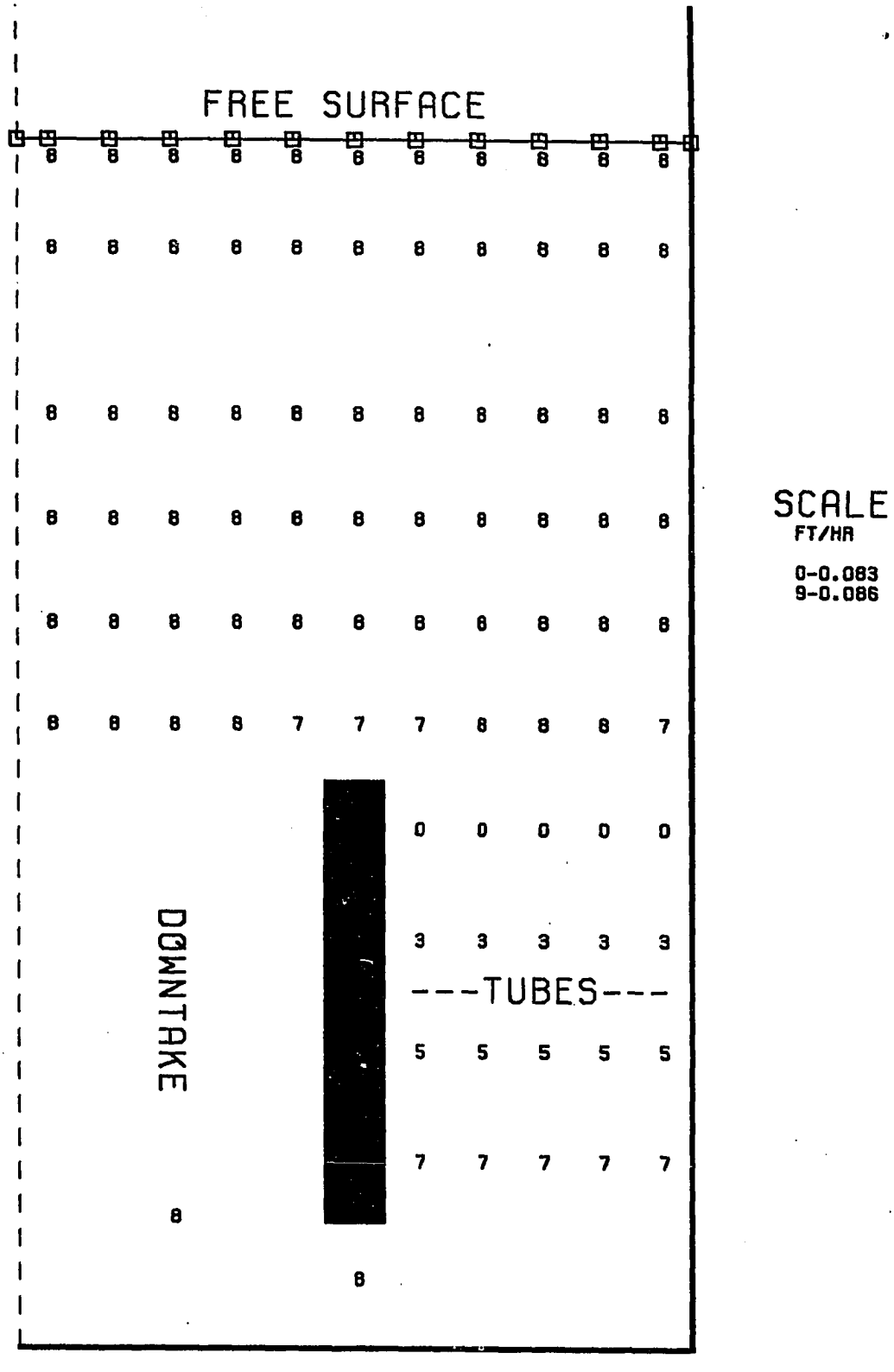


GROWTH PROFILE FIGURE 5.2.2 (10)
Effect of Increased Downtake Diameter



GROWTH PROFILE FIGURE 5.2.2 (11)

Effect of Increased Pressure and Reduced Supersaturation



GROWTH PROFILE FIGURE 5.2.2 (12)
Effect of Low Purity

5.3 COMPARISON OF PREDICTED TUBE VELOCITIES AGAINST LITERATURE

Verification of the fluid mechanics at this point is important because Pan recirculation and flow patterns are determined by density differences, which in turn, are a function of the thermodynamic state, which in turn, is a function of the flow of momentum and energy. Thus, verification of the flow pattern inherently verifies the temperature profiles which are important for calculating supersaturation profiles. However, difficulty arises in the verification of the model because data in the literature are not in sufficient detail and are few in number. Most of the data in the literature concerning flow profiles and velocity in the tubes are summarized in Honig (1963) and also in Hugot (1972).

In 1934, Webre measured the velocity in the tubes as a function of time during a batch production of C raw cane sugar by using two sensitive thermometers and a heat balance. Webre's work is summarized in Table 5.3.1. Webre calculated the velocity in the tubes from only sensible heat changes in the massecuite rising up the tubes neglecting any vaporization. Thus, his calculation over estimates the velocity in tubes when boiling occurs. With this in mind, the criticism of Webre's pan in the literature as being extremely fast for C massecuite may be justified.

Nonetheless, Webre's data as an order of magnitude illustration of the velocity in the tubes are useful. His data should be reasonably accurate for the later time intervals when boiling is less probable.

Hugot also summarizes some of the tube velocities reported by Clausen, for beet sugar, using a hot wire anemometer. Table 5.3.2 summarizes those data. The data are presented as typical tube velocities that vary with batch time and purity of the massecuite.

Comparing the data presented in Tables 5.3.1 and 5.3.2, gives the reader an idea of the typical velocities expected in an operating pan. As shown in the tables, typical tube velocities in a Vacuum Pan may vary from 5.5 FT./SEC. in the early portions of a high grade A massecuite batch to almost zero at the end of the low grade C massecuite batch. Since the velocities are very dependent on the pan design and the operating conditions, especially heat load, which are not available in Hugot or the original articles, there is no real basis for comparison against a simulated case. Therefore, these data are not in sufficient detail to be used for a detailed verification of the model simulation. Nonetheless, Webre's and Clausen's data do illustrate the velocity in a typical natural convecting Vacuum Pan and since the cases presented earlier in Table 5.2.3 do also, there is a basis for comparsion in terms of the order of magnitude.

Referring to Table 5.2.3, the predicted tube velocities vary from 1.0 FT./SEC. (Case 4), for a typical A or B grade massecuite to 0.1 FT./SEC. (Case 12), for a typical C massecuite. Since the model is not capable of simulating the early portions of the batch when the volume of massecuite is low and the volume fraction crystal is small, the velocities presented in Table 5.2.3 represent predictions resulting from conditions sometime after the first hour of operation of the Pan. This further restricts any comparisons of the predicted velocities against the literature. But, since the predicted velocities are within the correct range, this in itself is a favorable comparison. Reproducing the data in the literature is impossible without total specification of all the conditions concerning the experiment. Obviously, the data in the literature were not collected to verify a model such as this one because the essential information was omitted.

TABLE 5.3.1: WEBRE'S DATA

MASSECUITE PURITY		VELOCITY (FT/SEC)			
		1st hr.	2nd hr.	3rd hr.	6th hr.
C	60	1.53	0.63	0.15	0.01

TABLE 5.3.2: CLAUSEN'S DATA

MASSECUITE PURITY		VELOCITY (FT/SEC)	
		at the start	at the finish
A	96	3.3-5.5	0.72
B	82	1.08-0.72	0.02

5.4 NUMERICAL PROBLEMS AND HYDROSTATIC HEAD ASSUMPTION

As mentioned earlier, some numerical problems occured that prevented the simulation of the Pan during the early time intervals. This problem resulted because the explicit formulation of the mathematical model was unable to maintain a stable calculation when the flow is vigorously boiling, which is characteristic of the early time intervals of the batch. At the same time, it was observed that the hydrostatic head assumption that reduces the vertical momentum equation to a very simple form was in error because the inertial and the convective terms were obviously important. Instead of attempting a serious reprogramming effort it was, at this point, decided to proceed with the demonstration of the use of the model, but limit its application to times where the stability problem did not occur. In essence, this limits the applicability of the model to the later time intervals of the batch. This limitation can be thought of as not a serious one, because problems associated with operation of the Vacuum Pan occur because of inadequate mixing and recirculation which are characteristic of the later time intervals. Thus, limiting the application of the model to the later time intervals is just where the model is needed the most.

As already mentioned above, the hydrostatic head

assumption may not adequately describe the pressure profiles in an operating Vacuum Pan. The possibility of this inadequacy was also discussed when the mathematical model was derived. In order to capitalize as much as possible on the experience developed to this point in working with the program, preliminary work was done with the explicit solution sequence and the full vertical momentum equation to see if a stable numerical solution can be obtained of flows where the inertial and convective terms are important. The crystallizer, of course, was used for the study. With the full momentum equation, the solution became immediately unstable at any time step. After taking out the inertial term the solution was intially stable, but as the Pan heating continued a rapidly accellerating vortex formed in the Pan not allowing much convection to the surface so the hot liquid could boil. Soon afterwards, sufficient heat had accummulated to cause vigorous boiling and the solution became unstable. The diffusion terms were also included in the vertical momentum equation but their effect was small as demonstrated earlier. It can only be concluded that the one-step explicit method is not sufficient as a solution method when the inertial terms and the convective terms are important as the result vigorous boiling. Multi-step or an implicit method should clear up the problem because this would allow the

pressure to affect the vertical and radial momentum at the same time. Implicit and mixed implicit-explicit methods are characteristic of most two-phase flow calculations in the literature because of the stiffness caused by sudden changes in density. Therefore, it should not be expected that the explicit method would work. However, fundamental research needs to be done to devise an implicit method that is efficient and convergent.

CHAPTER 6

DYNAMIC GRID

One of the distinguishing problems with numerically solving free surface problems, or generically speaking, time dependent moving boundary problems, is the need for a dynamic grid. A grid that is able to detect a need for a different grid formation and change to accomadate the flow and the present conditions. Numerical schemes have been devised that accomplish this and have been published in the literature.

The MAC method, discussed in Chapter 4, is after a fashion dynamic, since, grid cells are added or taken away from the surface as the fluid dynamics suggest. The floating surface cell method used by Waldrop and Pitts, discussed in Chapter 4, is also dynamic since the surface cell heights change in response to the fluid dynamics. However, much more general development of the dynamic grid concept is developed in the literature. Both Pracht (1974) and Chan (1974) develop a dynamic grid capable of arbitrary grid movements, movements according to the Lagrangian View Point, or stationary grid arrangements. The development of such dynamic grids are based on simple reasoning which will be discussed below. However, application of this reasoning in combination with complex generalized numerical codes is difficult.

Since the goal of this research is not the development of a generalized code for modeling free surface flows, but, simply a numerical code that meets the needs for modeling the Vacuum Pan, the development of the dynamic grid below will be based on this premise. Nonetheless, extensions and generalizations could be done in future research efforts based upon the principles presented below.

The development of the dynamic grid system is constrained by Equation 4.1.1, the general property equation discussed in Chapter 4. Equation 4.1.1 is presented below.

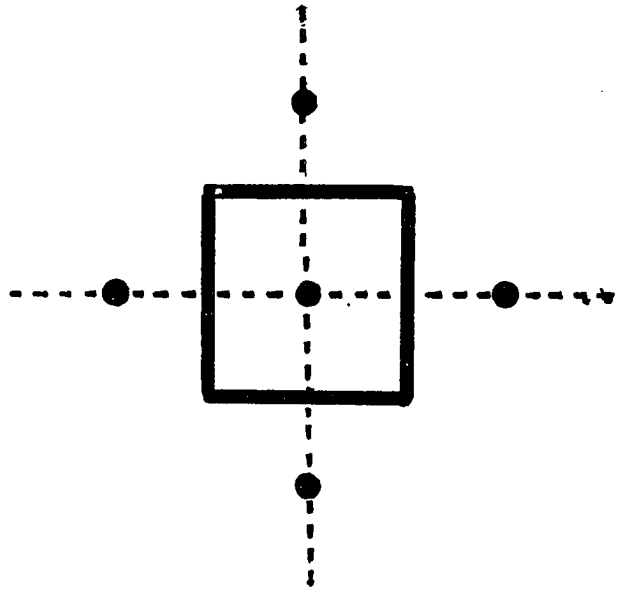
$$\frac{d}{dt}\int \rho \phi \, dV = - \oint \phi_F \cdot d\bar{A} + \int \phi_g \, dV \qquad 4.1.1$$

$$\phi_F = \rho U_{RB} \phi + \tilde{P}$$

In the development of the dynamic grid, the surface terms, compression forces and diffusion, are not effected or that is, do not change their form in Equation 4.1.1. These terms depend upon gradients that exist at the surface for the diffusion terms and the magnitude of the pressure for the compressive forces. However, translation of the cell boundaries does effect the convection of the general property into the volume. So the development of the dynamic grid must define this effect, as well as the effect of translation on cell volumes and boundary

areas.

Equation 4.1.1 expresses in a continuum sense, the conservation of ϕ in the volume of concern. The conservative principles do not restrict the size or shape of the volume in any way, therefore, Equation 4.1.1 also applies in a continuum sense to any arbitrary volume. Thus, Equation 4.1.1 also applies to the computation cell of the two-dimensional Pan Proper. The computation cell is presented below.



The computation center is located at the point (r_i, z_j). The boundaries are located as prescribed for this rectangular grid cell by the grid increments Δr_i and Δz_j. The radial cross-sectional area is given as a function of radial position by Equation 6.0.1, its volume by Equation 6.0.2, vertical areas by Equation 6.0.3.

$$A_r(i) = 2\pi r_i \, \Delta z \qquad 6.0.1$$

$$V(i) = 2\pi r_i \, \Delta r \, \Delta z \qquad 6.0.2$$

$$A_z(i) = 2\pi r_i \, \Delta r \qquad 6.0.3$$

Consider now that all the points in the computation cell are translated thru space at the same velocity, ($\mathfrak{V}_p$). This velocity ($\mathfrak{V}_p$) can be represented as the sum of its radial component (u_p) and vertical component (w_p). Because cell points in the cell are translating at the same velocity the boundary areas and volume of the cell do not change. But because of the translation, the convection of ϕ into the cell is effected by the relative motion of the cell boundaries to the fluid motion. The convection of the general properties is expressed by the integral below, Equation 6.0.4.

$$\oint \rho U_{RB} \, \phi \cdot d\bar{A} \qquad 6.0.4$$

Where U_{RB} expresses this relative motion. This relative motion is described mathematically below, by Equation 6.0.5.

$$U_{RB} = U - \mathfrak{V}_p \qquad 6.0.5$$

Equation 6.0.5 can be broken down into its radial component, Equation 6.0.6, and its vertical component, Equation 6.0.7.

$$u_{RB} = u - u_p \qquad 6.0.6$$

$$w_{RB} = w - w_p \qquad 6.0.7$$

Now consider the possibility of the distortion of the cell. In other words, each point within the cell may be moving at different velocities, therefore, the cell boundaries and volume may change as the result of this distortion. Nonetheless, Equation 4.1.1 still describes the conservation of the general property. Likewise, Equation 6.0.4 still represents the convection of the general property into the cell. Now in terms of the computation effort if $\mathcal{V}_p$ equals U then there is no convection of the general property into the cell, and Equation 4.1.1 is said to represent the Lagrangian point of view, i.e., the coordinate system moves the fluid. In contrast, if $\mathcal{V}_p = 0$, then Equation 4.1.1 is said to represent the Eulerian point of view, i.e., the cell is fixed in space. However, the conservation principles do not limit the situation to these two cases. Therefore, $\mathcal{V}_p$ may be arbitrary specified to meet pertinent computation purposes.

The purpose of the dynamic grid system proposed here is to maintain, for a constant number of computational cells, a positive volume in all of the computaional cells in the face of volume changes in the Pan Proper (the computational space). The methodology for adjusting the grid is based on the assumption that the average surface cell height is maintained constant and the average surface cell height is sufficient to prevent negative heights resulting from surface curvature. Furthermore, the surface is always assumed to be contained in the Pan Proper. Also, the radial grid increments remain constant for computation convenience and the inner vertical grid increment remains uniform for computation convenience but changes in response to volume changes in the Pan. This state is easily accomplished by letting (u_p) equal to zero but letting (w_p) change for the inner cells according to Equation 6.0.8.

$$w_p(z_j) = \frac{z_j}{z_{ic}} \frac{d\bar{z}}{dt} \qquad 0 < z_j < z_{ic} \qquad 6.0.8$$

Where ($\bar{z}$) is the average level in the Pan Proper, (z_{ic}) is the inner cells boundary height, and (z_j) is the vertical position in the Pan Proper. In terms of the computational grid for the Pan Proper, (z_j) is calculated via Equation 6.0.9, for the cell center and via Equation 6.0.10, for the vertical cell boundaries.

$$z_j = \Delta z(2j-1)/2 \qquad j = 1,2...jmax \qquad 6.0.9$$

$$z_j = \Delta z\ j \qquad j = 0,1,2...jmax \qquad 6.0.10$$

The vertical grid increment is defined by Equation 6.0.11, where jmax is the number of grid cells in the inner grid.

$$\Delta z = (\bar{z}-\bar{h})/jmax \qquad 6.0.11$$

Since the vertical grid increment (Δz) may change with time, but as mentioned earlier, the average surface height is to remain constant in time, therefore, upon differentiating Equation 6.0.11 with respect to time, Equation 6.0.12 results.

$$\frac{d\,\Delta z}{dt} = \frac{d\bar{z}}{dt}/jmax \qquad 6.0.12$$

Equation 6.0.12 can then be integrated with respect to time to give the vertical grid increment. Since the radial cross-sectional areas and the cell volume are related to the vertical increment, these quantities will change in time.

Although, to this point the discussion has been limited to the inner grid cell, the development also

applies to the surface cells. Equation 6.0.13 is the vertical velocity of each point in the surface cell.

$$w_p(z_j) = \frac{(z_j - z_{ic})}{h_i} \frac{dh_i}{dt} + \frac{d\bar{z}}{dt} \qquad 6.0.13$$

$$0 < z_j - z_{ic} < h_i$$

Where (h_i) is the surface cell height of the (i) radial position.

Since the discrete analog of the Equation 4.1.1, derived in Chapter 4, are derived specifically to include all the dynamic terms, applying the above equations in combination with the physics of the Pan, allows a computational set of equations to be specified that will adjust for volume changes in the Pan.

CHAPTER 7

SUMMARY AND CONCLUSIONS

In the preceding chapters, the reader has been introduced to the analysis of lumped particle systems and distributed particle systems. A distributed particle system as opposed to a lumped well mixed tank approach is needed when local disturbances or conditions have a significant effect on the resulting crystal size distribution (CSD). Such a circumstance might well describe the conditions in a Vacuum Pan Sugar Crystallizer. Of course, the distributed particle analysis has need of distributed velocity and growth profiles. Thus, the particle equation must be solved simultaneously with a distributed mathematical model of the fluid dynamics. The only recourse to this method is to use empiricism based on experimental data, this direction was taken by Wright (1974). But this approach does little in the way of helping to design control systems for Pans or in the design of Pans. This type of empiricism is dependent on the Pan and the operating conditions. The empiricism also lacks information that is needed to decide what kind of instrument to be used and how many and where it should be placed and what kind of effects Pan design and operating conditions have on the ability of the control system to meet a target CSD. The approach used here has

been to develop a mathematical model based on the fundamental laws of fluid dynamics to supply the needed information to a distributed particle balance. The distributed model would, by its nature, supply the essential information the empiricism lacks.

The derivation of the model introduces the reader to the basics of two-phase fluid flow. The later discussion of the numerical methods introduces the reader to the state of the art of numerical methods in two-phase flow and their applications. The numerical solution scheme for free surface problems was developed by Waldrop (1972), and is explicit in nature as opposed to mixed implicit-explicit methods used in the literature. The application of this solution scheme, presented in detail in Chapter 4, is completely new. This method was chosen over complicated methods because of its simplicity. The desire here was to use the most efficient code for the particular problem so the entire batch of several hours might be simulated. While previous work has been done by Pitts (1976) and Waldrop (1972) here at Louisiana State University on incompressible flow with a free surface, the finite difference methods used were very inconsistent and the surface cells were not treated properly. Therefore, quite a bit of fundamental research had to be done to make the finite difference equations consistent throughout the grid system and between

equations. This work is in addition to work done in designing the two-phase calculations and finding a method of removing the vapor from the Pan that is consistent with the homogeneous model. Additional work was done in the development of a much needed dynamic grid system without which an entire batch crystallization simulation cannot be attempted in a distributed system. The resulting numerical method is conservative and transportive and does not need a strong artifical diffusion to prevent numerical wandering of the numbers, in fact, needs no diffusion in the momentum and energy calculation to prevent numerical wandering of the numbers. This fact is demonstrated with a sensitivity analysis of the thermal diffusivity, Cases 2 and 3, in Table 5.1.1. The need for diffusion to prevent the wandering of the numbers is a sign that the finite differencing method does not satisfy all the equations simultaneously. Many times this numerical wandering of the numbers is mistaken for numerical instability. The differencing methods used by Pitts and Waldrop have this problem throughout the grid system and especially in the surface cells. The finite difference method developed in this work is conditionally stable as expected for explicit solution sequence, but its increased stability is characteristic over the methods in earlier works here at LSU. Also, the surface calculation is done with an implicit

tri-diagonal matrix solver. However, the model does have limitations associated with the assumptions made in the derivation of the mathematical model and when the numerical model was derived, these problems were discussed earlier.

Studies using the model to perform sensitivity analysis of the solution to the thermal diffusivity and demonstrate the use of the program to analyze pan design and operating conditions on pan performance are presented in the previous pages. The effect of pan design and operating conditions is seen to be significant, suggesting that the model could be used to aid in pan design and increasing the performance of existing pans. This type of analysis has never been attempted for a Vacuum Pan Sugar Crystallizer. The parameters used to measure the effect variations in pan design and operating conditions were changes in the growth and velocity profiles, the difference between the maximum and minimum supersaturation, and the recirculation rate. These of course, affect the product CSD tremendously. The most significant variations of the operating conditions studied were, the volume fraction crystals, pan level, heat load, and pan pressure. The most significant variations of pan designs studied were, the flare design over the straight walled pan and heat transfer area.

The sensitivity studies varying pan design demonstrate that contrary to some statements in the literature, large downtakes in excess of 40% of the Calandria diameter are not

needed, especially when heat transfer area is sacrificed. These studies also show that simple design changes such as the flare design may adversely effect the CSD because of the effect on the circulation patterns in the pan. The flare design causes a vortex zone or eddy near the wall that extends from the surface to the Calandria. This vortex may trap crystals for large enough periods of time to cause the crystals in this area to have a significantly different average size and thus, contribute to the variance of the product CSD.

The model demonstrates that the ability of the pan to transfer heat through its Calandria is one of the most important parameters to be considered when judging the performance of a Vacuum Pan. Good heat transfer is synonymous with good circulation, and good circulation is an indication that the pan will produce a uniform CSD. Therefore, it can only be concluded that development of a good correlation for the heat transfer coefficient in the pan would be a significant contribution to this research. The heat transfer correlation should be sensitive to the fluid dynamics as well as the physical properties.

The sensitivity studies show in all cases that there are significant growth profiles throughout the Pan. This fact suggests that the utility of multiple instrument probes to measure local supersaturation could prove great. Thus, the modern approach to use multiple instrument

probes in the Pan seems justified.

For the most part, the importance of the various pan designs and operating conditions mentioned above, at least to an experienced sugar boiler, is no revelation. However, the advantage the model offers is that quantitative effects of these design and operating conditions on the growth and velocity profiles and recirculation are calculated. These are essential parts of the analysis of the effects of pan design and operating conditions on the CSD based on a distributed population balance as discussed in Chapter 2. Thus, the model developed and demonstrated in this research must be looked upon as a stepping stone to bigger and better things. A model of this type is essential as a research tool and could aid in the development of a more efficient Vacuum Pan.

CHAPTER 8

RECOMMENDATIONS

To this point, the development of a mathematical model for a Vacuum Pan Sugar Crystallizer is not complete. The success of the present model in predicting natural convecting flows is evident. This success suggests that further research in modeling the Crystallizer should be continued. The recommendations for continued research are several fold and are experimental as well as computational. The recommendations are as follows:

(1) Basic computational research to develop multi-step or implicit numerical solution methods, to remedy the stability problems discussed earlier. The formulation of the mathematical model should not include the hydrostatic head assumption. Instead, the full vertical momentum equation should be programmed.

(2) Basic computational research to reduce the execution time for the dynamic flow model. This could be done by modifying the equations to reduce stiffness, thus, allowing bigger time steps to be taken. Elimination of all the diffusion terms might be considered to reduce the number of executions. Modification of the equations might be done by elimination of some of the dynamic terms, which tend to follow the oscillatory nature

of the two-phase flow transients, rather than the underlying quasi steady state nature of the Pan. The dynamics of which variables to be ignored and what method of converging the solution set, considering the free surface, should be part of the research.

(3) The particle equations should be included in the mathematical and numerical formulation, if the quantitative effects of Pan design and operation on the resulting CSD are desired.

(4) Experimental work to develop correlations for the local heat transfer coefficients and pressure drop in a crystallizer tube. This work could also involve modeling the crystallizer tube.

(5) Experimental measurement of velocity profiles and recirculation rates to aid in verification of future computational efforts in modeling the crystallizer.

The recommendations listed above directly extend the present work. However, the computation methods and literature cited in this dissertation are applicable to other industrially important problems. Further development of methods for two-phase flow would be beneficial because such methods are very marketable in industry today.

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NOMENCLATURE

A	($FT.^2$)	Area
$A_r(i)$	($FT.^2$)	Area viewed from radial direction at the i position
$A_z(i)$	($FT.^2$)	Area viewed from vertical direction at the i position
AREAT	($FT.^2$)	Area for heat transfer
B	($NO./FT.^4$)	Nucleation Rate Distribution Function
B_o	($NO./FT.^4$)	Nucleation Rate
BPE	(F)	Boiling Point Elevation
BRIX		Mass fraction sucrose and impurities in massecuite
C	(LB.)	Mass of crystal
CP	(BTU/LB.-F)	Heat capacity of mixture
CPW	(BTU/LB.-F)	Heat capacity of water
CSD	($FT.^{-1}$)	Crystal Size Distribution
$\frac{D}{Dt}$		Substantial Derivative
D_c	(FT.)	Diameter of Calandria
D_{dwn}	(FT.)	Diameter of Downtake
D_t	(FT.)	Diameter of Tubes
DPDT	(FT./SEC.)	Velocity of Cell
E	($LB./SEC.-FT.^2$)	Evaporation Rate Flux
EACT	($\frac{KC}{g\text{-}MOLE}$)	Activation Energy

ECOEFF	(LB./FT.^{2}-SEC.)	Evaporation Coefficient
ER	(LB./SEC.)	Evaporation Rate
F	(LB./SEC.)	Feed Rate
F_B	(LB.-FT./SEC.^{2})	Body Force
FR	$\left(\frac{\text{LB.-FT./SEC.}^2}{\text{FT.}^3}\right)$	Pressure drop due to friction
g	(FT./SEC.^{2})	Acceleration due to gravity
G	(FT./SEC.)	Growth Rate
h	(FT.)	Surface Cell Height
H	(BTU/LB.)	Enthalpy
HF	(BTU/LB.)	Enthalpy of Feed
HL	(BTU/LB.)	Enthalpy of Liquid
HV	(BTU/LB.)	Enthalpy of Vapor
IMP	(LB.)	Mass of impurities
k_G	(FT./SEC.)	Growth Rate Constant
k_G^o	(FT./SEC.)	Specific Growth Rate
L	(FT.)	Crystal Size
$\bar{L}$	(FT.)	Average Crystal Size
M_k		kth moment of η
N_c		Number of Crystals
NTUBES		Number of Tubes
OS		Oversaturation
P	$\left(\frac{\text{LB.-FT./SEC.}^2}{\text{FT.}^2}\right)$	Pressure

PR	$(\frac{\text{LB.-FT./SEC.}^2}{\text{FT.}^2})$	Reference Pressure
P	(LB.-FT./SEC.)	Dynamic Momentum
POA	(FT.^{-1})	Perimeter of Tubes divided by the area for flow
Q	$(\text{FT.}^3/\text{SEC.})$	Volumetric Flow Rate
r	(FT.)	Radial Position
R_{dwn}	(FT.)	Radius of Downtake
R_g	(KC/g-MOLE-R)	Gas Law
S	(LB.)	Mass of Sucrose
SAT	(LB./LB.)	Saturation mass of sucrose per 100 pounds of water
SFSMTH	$(\text{FT.}^2/\text{SEC.})$	Surface Diffusivity
SS		Supersaturation
t	(SEC.)	Time
T	(F)	Temperature
TMASS	(LB.)	Total Mass
TSTEAM	(F)	Temperature of Steam
TUBED	(FT.)	Tube Diameter
TUBEH	(FT.)	Tube Height
TW	(F)	Temperature of Water
u	(FT./SEC.)	Radial Velocity Component
u_{RB}	(FT./SEC.)	Radial Velocity relative to boundary of cell
U	(FT./SEC.)	Velocity Vector
U_{RB}	(FT./SEC.)	Velocity Vector relative to boundary motion

UPOA	(BTU/SEC.-FT.^{3}-F)	Overall coefficient times perimeter divided by area for flow
UU	(BTU/SEC.-FT.^{2}-F)	Overall heat transfer coefficient
V	(FT.^{3})	Volume
VCL		Volume Ratio of Crystal Volume to Liquid Volume
w	(FT./SEC.)	Vertical Velocity Component
w_{RB}	(FT./SEC.)	Vertical Velocity Relative to Cell Boundary
w_s	(FT./SEC.)	Velocity of Surface
w_v	(FT./SEC.)	Velocity of Vapor
W	(LB.)	Mass of Water
W_V^*	(FT./SEC.)	Maximum Vapor Slip Velocity
x		Mass Fraction
XCP		Mass Fraction of Crystal in Pan
XIMP		Mass Fraction of Impurity in Pan
XIMF		Mass Fraction of Impurity in Feed
XL		Mass Fraction of Liquid
XSP		Mass Fraction of Sucrose in Pan
XSF		Mass Fraction of Sucrose in Feed
XWP		Mass Fraction of Water in Pan
XWF		Mass Fraction of Water in Feed
z	(FT.)	Vertical Position

GREEK

α	(FT.^{2}/SEC.)	Thermal Diffusivity
β	(F^{-1})	Coefficient of Thermal expansion
β_c	(BRIX^{-1})	Coefficient of Concentration
γ		Volume fraction
η	(NO./FT.^{4})	Crystallizer Number Density Function
Δr	(FT.)	Radial increment
Δt	(SEC.)	Time increment
Δz	(FT.)	Vertical increment
κ	(BTU/SEC.-FT.-F)	Thermal Conductivity
μ	(LB./FT.-SEC.)	Viscosity
μL	(LB./FT.-SEC.)	Viscosity of molasses
ν	(FT.^{2}/SEC.)	Kinematic Viscosity
ρ	(LB./FT.^{3})	Density
ρL	(LB./FT.^{3})	Density of liquid
ρLS	(LB./FT.^{3})	Density of liquid and solid mixture
ρR	(LB./FT.^{3})	Reference Density
ρV	(LB./FT.^{3})	Density of vapor
ρVR	(LB./FT.^{3})	Reference density for vapor
σ^2	(FT.^{2})	Variance of Crystal Size Distribution
$\boldsymbol{\tau}$	$\left(\frac{\text{LB.-FT./SEC.}^2}{\text{FT.}^2}\right)$	Stress Tensor
ϕ	(property/LB.)	General Property

ϕ_c	(BTU/SEC.)	Generation of energy due to Crystallization
ϕ_g	$(\frac{\text{property}}{\text{SEC.-FT.}^3})$	Generation of General Property

APPENDIX I

LISTING OF COMPUTER PROGRAM

This appendix presents a listing of computer program modeling the Vacuum Pan. The mathematical model and numerical methodology are presented in Chapters 4 and 5 of the main text. Comment cards are used throughout the listing to aid understanding. For as much as possible the symbols used in the computer programming are the same as used in the text.

All data needed for execution of the program are obtained upon execution of SUBROUTINE PRELIM. If a cold start is selected, initialization of the computational matrix is accomplished through statements in SUBROUTINE PRELIM. If a restart is selected, the computational matrix is initialized from a sequential file. Non-dimensionalization of the computational matrix is accomplished through statements in SUBROUTINE PRELIM.

At the completion of the run the computation matrix is dumped into a sequential file. This allows the restart feature to be executed.

After the program has executed the proper number of time steps, the program tabulates the computational matrix, as well as a brief summary of the run. Intermediate tabulation of the computational matrix is possible if desired, but, may also result if a

computation error occurs.

Separate programs are used when velocity or growth profiles are needed. These programs access the same sequential file needed to supply the restart capability to obtain the computation matrix. A listing of these programs are not included.

A listing of the computer program is now presented.

```
C-----                                                                  00010001
C-----  MAIN PROGRAM. MOTIVE FORCE FOR CALCULATION.                     00010002
C-----                                                                  00010003
      IMPLICIT REAL*8(A-H,O-Z)                                          00010004
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                 00020000
      DIMENSION ZPARS(5),ZPARV(4),ZPARH(8),ZPARG(9),ZPART(3)            00030000
      DIMENSION ZPARCP(4),ZPARBP(2),ZRATIO(3)                           00040000
      REAL*8 IMP(2)                                                     00050000
      COMMON/ BLOCK  /  ERIXFF, PURFF,TEMPFF,                           00060000
     1       VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                 00070000
      COMMON/JOBRUN/ IRUN(3)                                            00080000
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,EPE,VRATIO         00090000
      COMMON/ CONECT/ HBNDS(30),DBNDS(30),TBNDS(30),QJCAL               00100000
      COMMON/MOVE   / DPDT(30)                                          00110000
      COMMON/FORCE/ PUMPDP                                              00120000
      COMMON/INOUT/IN,IOUT                                              00130000
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       00140000
     1,            F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)     00150012
     2,            TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)       00160000
     3,            SSMAX, SSMIN                                         00170000
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, ENVINT, AQFLUX               00180011
      COMMON/FLAG/ IWSTRT, IFLAG1, IFLAG2                               00190000
      COMMON/REAL/ RTIME, TCONST                                        00200000
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVCL, WHEIG                      00210000
      COMMON/DIMEM/ U(2,30,30), W(2,30,30), T(2,30,30), WW(30,30)       00220000
      COMMON/DIMEN1/ P(30,30), PBIP1, PBIM1                             00230000
      COMMON/IPHASE/ ENTH(2,30,30), DEN(2,30,30)                        00240000
      COMMON/GRID/ DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ     00250000
     1,            DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ       00260000
     2,            DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO      00270000
     3,            DZODTO                                               00280000
      COMMON/PROPTY/ RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA             00290000
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                00300000
     2,              HVINV,DELHLV,DENSTY                                00310000
      COMMON/COORD/ R(30),Z(30),RINV(30),RH(30)                         00320000
      COMMON/LIMITS/ IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT  00330000
```

```
1,              NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1                  00340000
 COMMON/STEP/ MN,MO,N                                                   00350000
 COMMON/SIZE/ H,RAD,HMAX                                                00360000
 COMMON /AREAP/ DV(30),DVOA(30)                                         00370000
 COMMON/BOUND/ IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                  00380000
1,             IDWNP1,IDOWM1                                           00390000
 COMMON/CHEST/ UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH       00400000
1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                 00410000
2,NCALP1                                                                00420000
 COMMON/FLOW1/ DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT           00430000
1,             DDDZDT(30,30),DDCDT(10)                                  00440000
 COMMON/AVPART/AVERNN(2),AVERLL(2)                                      00450000
 COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                        00460000
1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                     00470000
 COMMON/ENTLIM/ XVLIM                                                   00480000
 COMMON/VAPDEN/ PRESRF,RHOVR                                            00490000
 COMMON/LUMBT/ WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                  00500000
1,             WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                     00510000
2,             UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2)          00520000
3,             HCALAV(2),WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)        00530000
 COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)             00540000
1,              CALP(10,2)                                              00550000
 COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                     00560000
1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8                   00570000
1,              ENTHFR, FFLUXU                                          00580000
 COMMON/ EMPEQ/ SLIPV, EXPV                                             00590000
 COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)              00600000
 COMMON/ EQUTON / RATCR                                                 00610000
 COMMON / PARS/   PARS1, PARS2, PARS3, PARS4, PARS5                     00620000
 COMMON / SPARS/ SPARS1, SPARS2, SPARS3, SPARS4, SPARS5                 00630000
 COMMON / PARV/ PARV1, PARV2, PARV3, PARV4                              00640000
 COMMON / SPARV/ SPARV1, SPARV2, SPARV3, SPARV4                         00650000
 COMMON / PARH/  PARH1, PARH2, PARH3, PARH4,                            00660000
&                PARH5, PARH6, PARH7, PARH8                             00670000
 COMMON / SPARH/ SPARH1, SPARH2, SPARH3, SPARH4,                        00680000
&                SPARH5, SPARH6. SPARH7, SPARH8, SPARH9                 00690000
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```
      COMMON / PARG/ PARG1, PARG2, PARG3, PARG4,                        00700000
     &               PARG5, PARG6, PARG7, PARG8, PARG9                  00710000
      COMMON / SPARG/ SPARG1, SPARG2, SPARG3, SPARG4,                   00720000
     &                SPARG5, SPARG6                                    00730000
      COMMON / PART/ PART1, PART2, PART3                                00740000
      COMMON / SPART/ SPART1, SPART2, SPART3                            00750000
      COMMON / PRATIO/ PARR1, PARR2, PARR3                              00760000
      COMMON / PARCP/ PRCP1, PRCP2, PRCP3, PRCP4                        00770000
      COMMON / PARBP/ PRBP1, PRBP2                                      00780000
      COMMON / SPRATO/ SPARR1, SPARR2, SPARR3                           00790000
      COMMON / SPARCP/ SPRCP1, SPRCP2, SPRCP3, SPRCP4                   00800000
      COMMON / SPARBP/ SPRBP1, SPRBP2                                   00810000
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/         00820015
      EQUIVALENCE (ZZZZ,WDWNJP)                                         00830000
      EQUIVALENCE (ZZZC,CALW)                                           00840000
      EQUIVALENCE (ZPARS,PARS1)                                         00850000
      EQUIVALENCE (ZPARV,PARV1)                                         00860000
      EQUIVALENCE (ZPARH,PARH1)                                         00870000
      EQUIVALENCE (ZPARG,PARG1)                                         00880000
      EQUIVALENCE (ZPART,PART1)                                         00890000
      EQUIVALENCE (ZPARCP,PRCP1)                                        00900000
      EQUIVALENCE (ZPARBP,PRBP1)                                        00910000
      EQUIVALENCE (ZRATIO,PARR1)                                        00920000
C                                                                       00930000
      CALL PRELIM                                                       00940000
      CALL OUTPUT                                                       00950000
      CALL OUTALL                                                       00960000
      CALL BOUNDY                                                       00970000
C                                                                       00980000
C     BIG LOOP STARTS HERE                                              00990000
C                                                                       01000000
      MOO=MO                                                            01010000
      MO=MN                                                             01020000
      MN=MOO                                                            01030000
      DO 999 N=1,NMAX                                                   01040000
      RTIME=RTIME+TCONST*DT                                             01050000
```

```
C                                                                       01060000
C        CALCULATE NEW RADIAL VELOCITIES,ENTHALPIES,DENSITIES           01070000
C        AND TEMPERATURES ABOVE THE CALANDRIA                           01080000
C                                                                       01090000
      CALL HUNEW                                                        01100000
C                                                                       01110000
C           CALCULATION OF NEW ENTHALPIES, DENSTIES, TEMPERATURES,      01120000
C           AND VELOCTIES FOR CALANDRIA AND BOTTOM                      01130000
C                                                                       01140000
      CALL LOOP                                                         01150000
C                                                                       01160000
C           SET BOUNDARY CONDITIONS BETWEEN CALANDRIA AND PAN PROPER    01170000
C                                                                       01180000
      CALL BOUNDY                                                       01190000
C                                                                       01200000
C           CALCULATION OF AVERAGE CONDITIONS IN PAN                    01210000
C                                                                       01220000
      CALL AVERGE                                                       01230000
C                                                                       01240000
C           CALCULATE VAPOR RATES FROM FREE SURFACE                     01250000
C                                                                       01260000
      CALL CALVAP                                                       01270000
C                                                                       01280000
C           USE TO CHANGE MANIPULATED AND LOAD VARIABLES                01290010
C                                                                       01300010
      CALL CONTRL                                                       01310010
C                                                                       01320010
C           WELL MIXED TANK CALCULATIONS                                01330010
C                                                                       01340010
      IF(IWSTRT.GT.0) CALL WMIXT                                        01350010
C                                                                       01360000
C           MOVE GRID POINTS                                            01370000
C                                                                       01380000
      CALL REZONE                                                       01390000
C                                                                       01400000
C           CALCULATE NEW VERTICAL VELOCITIES                           01410000
```

```
C                                                                       01420000
      CALL CONTIN                                                       01430000
C                                                                       01440000
C                                                                       01450000
C          CALACULATE RATE OF CHANGE OF FREE SURFACE POSITION           01460000
C          AND LOCATE FREE SURFACE POSITION                             01470000
C                                                                       01480000
      CALL CONVSF                                                       01490000
C                                                                       01500000
C          CALCULATE PRESSURE PROFILE                                   01510000
C                                                                       01520000
      CALL PRES                                                         01530000
C                                                                       01540000
C          ONE-D PRESSURE CALCULATIONS THROUGH CALANDRIA                01550000
C          AND DOWNTAKE                                                 01560000
C                                                                       01570000
      CALL PRESSC                                                       01580000
C                                                                       01590000
CC                                                                      01600000
C                                                                       01610000
      IF(N/NSTART.EQ.0) GO TO 91                                        01620000
      IF(N/NPRINT*NPRINT.EQ.N) CALL OUTPUT                              01630000
      IF(N/NEAR*NBAR.EQ.N) CALL OUTALL                                  01640000
C                                                                       01650000
 91   CONTINUE                                                          01660000
      MOO=MO                                                            01730000
      MO=MN                                                             01740000
      MN=MOO                                                            01750000
 999  CONTINUE                                                          01760000
C                                                                       01770000
C  BIG LOOP ENDS HERE                                                   01780000
C                                                                       01790000
      MOO=MO                                                            01800000
      MO=MN                                                             01810000
      MN=MOO                                                            01820000
```

```
      WRITE(6,1112)  IOUT                                                    01830000
      H=HH(MN)                                                               01840000
 1112 FORMAT(1X,'NOW WRITTING DATA CNTO UNIT ',I2)                           01850000
      DIMKV  = HMAX*DSQRT(HMAX*GR)                                           01860005
      SFSMTH = SFSMTH*DIMKV                                                  01870005
      VART   = VART*DIMKV                                                    01880005
      ALPHA  = ALPHA*DIMKV                                                   01890006
      F      = F/TCONST*3600.0D0                                             01900013
      UU     = UU/TCONST*3600.0D0                                            01910013
      TSTEAM = TSTEAM/BETA+TZERO                                             01920000
      RATCR  = RATCR/TCONST*3600.0D0                                         01930013
      PRESRF = PRESRF*DENSTY*HMAX/144.0D0                                    01940000
      RHOVR  = RHOVR*DENSTY                                                  01950000
      SLIPV  = SLIPV*DSQRT(GR*HMAX)                                          01960007
C----                                                                        01970000
C----  OUTPUT TO DISK                                                        01970001
C----                                                                        01970002
      REWIND ICUT                                                            01970003
      WRITE(IOUT,1111) U,W,T,P,ENTH,DEN,DUDT,DEDT,ZZZZ,WW,HCDT               01980000
     1,ZZZC,DHDT,SURFAC,H,RAD,HMAX,BTDUDT,BTDEDT                             01990000
     1,DDDZDT,DDCDT                                                          02000000
     2,EM,S,IMP,C,Q,AVERT,HH,F,BRIXFF,PURFF,TEMPFF                           02010008
     3,G,TMASS,WATER,AVERD                                                   02020008
     4,AVERH,RTIME,VOLSCH,RADSQ,VOLC,WVOL,WHEIG,AREAT                        02030000
     5,DT,DR,DZ,CDZ,DDZDT,SURFDT                                             02040005
     6,BETA,AVERNN,AVERLL                                                    02050000
     7,DENSTY,SLIPV,EXPV,VART,HR,ALPHA,SFSMTH                                02060007
     X,UU,UA,TUBEH,POA,UPOA,TUBED,CALANH,TSTEAM,TZERO                        02070000
     X,FRAT,BOTTH,RATCR                                                      02080000
     X,RHOVR,PRESRF,DELDDB,BRIXR                                             02090000
     X,TOTALH,XSP,XIP,XCP,XWP,PBIP1,PBIM1                                    02100000
     1,ZPARS,   ZPARV,   ZPARH,   ZPARG,   ZPART                             02110000
     2,ZPARCP,   ZPARBP,   ZRATIO                                            02120000
      WRITE(IOUT,1113) IMAX,JMAX,IRIGHT,ILEFT,IDOWN,MN,MO                    02130000
     9,NTUBES,NCAL,IRUN                                                      02140000
 1111 FORMAT(250A8,250A8,250A8,250A8,250A8,250A8,250A8,250A8,250A8           02150000
```

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02160000
02170000
02180000
02190000
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      1,133A8)
 1113 FORMAT(19A4)
      STOP
      END
```

```
      SUBROUTINE AVERGE                                                 02190003
C----                                                                   02190004
C---- PREFORMS AVERAGING OF PERTINENT VARIABLES                         02190005
C----                                                                   02190006
      IMPLICIT REAL*8(A-H,O-Z)                                          02190007
      DIMENSION ZZZ2(2,20),ZZZC(10,2,5)                                 02190008
      REAL*8 IMP(2)                                                     02190009
      COMMON/BOTTOM/ VOLUP, AFIWU, AFLWD, ABOAFD, ABOAFU                02190010
     1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8              02190011
     1,              ENTHFR, FFLUXU                                     02190012
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190013
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190014
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190015
     3,           SSMAX, SSMIN                                         02190016
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               02190017
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      02190018
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02190019
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                02190020
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          02190021
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190022
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190023
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190024
     3,          DZODTO                                                02190025
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02190026
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190027
     2,             HVINV,DELHLV,DENSTY                                02190028
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190029
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190030
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             02190031
      COMMON/STEP/MN,MO,N                                               02190032
      COMMON/SIZE/H,RAD,HMAX                                            02190033
      COMMON /AREAP/DV(30),DVOA(30)                                     02190034
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                 02190035
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN              02190036
     1,IDWNP1,IDOWM1                                                    02190037
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190038
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1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                  02190039
2,NCALP1                                                                 02190040
 COMMON /FLOW/DWT                                                        02190041
 COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT             02190042
1,DDDZDT(30,30),DDCDT(10)                                                02190043
 COMMON/AVPART/AVERNN(2),AVERLI(2)                                       02190044
 COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                         02190045
1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                      02190046
 COMMON/ENTLIM/XVLIM                                                     02190047
 COMMON/VAPDEN/PRESRF,RHOVR                                              02190048
 COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                    02190049
1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                                   02190050
2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)              02190051
3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                                02190052
 COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)              02190053
1,CALP(10,2)                                                             02190054
 COMMON/ EMPEQ/ SLIPV, EXPV                                              02190055
 COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)               02190056
 DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/               02190057
 EQUIVALENCE (ZZZZ,WDWNJP)                                               02190058
 EQUIVALENCE (ZZZC,CALW)                                                 02190059
 DELT=0.0                                                                02190060
 RNEW=0.0                                                                02190061
 COMP2=0.0                                                               02190062
 HNEW=0.0                                                                02190063
 SUMG=0.0                                                                02190064
 SSMIN=100.0                                                             02190065
 SSMAX=0.0                                                               02190066
 DO 80 I=2,IMAX                                                          02190067
 DDVI=DV(I)                                                              02190068
 SURFI=SURFAC(I)                                                         02190069
 DDDVI=DDVI*SURFI/DZ                                                     02190070
TNEW=T(MN,I,JMAXP1)                                                      02190071
 SS    = SUPERS(TNEW,XSP(MO),XIP(MO),XWP(MO))                            02190072
IF(SS.GT.SSMAX) SSMAX=SS                                                 02190073
IF(SS.LT.SSMIN) SSMIN=SS                                                 02190074
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      SUMG = SUMG+GROWTH(TNEW,SS,XIP(MO),XWP(MO))*DDDVI                 02190075
      DNEW=DEN(MN,I,JMAXP1)                                             02190076
      DOLD=DEN(MO,I,JMAXP1)                                             02190077
      DHNEW=ENTH(MN,I,JMAXP1)                                           02190078
      DHOLD=ENTH(MO,I,JMAXP1)                                           02190079
      COMP2=COMP2+DDDVI                                                 02190080
      DELT=DELT+TNEW*DDDVI                                              02190081
      HNEW=HNEW+DHNEW*DDDVI                                             02190082
      RNEW=RNEW+DNEW*DDDVI                                              02190083
      DO 80 JJ=1,JMAX                                                   02190084
      J=JMAXP1-JJ                                                       02190085
      DHNEW=ENTH(MN,I,J)                                                02190086
      DHOLD=ENTH(MO,I,J)                                                02190087
      TNEW=T(MN,I,J)                                                    02190088
      SS   = SUPERS(TNEW,XSP(MN),XIP(MN),XWP(MN))                      02190089
      IF(SS.GT.SSMAX) SSMAX=SS                                          02190090
      IF(SS.LT.SSMIN) SSMIN=SS                                          02190091
      SUMG = SUMG+GROWTH(TNEW,SS,XIP(MN),XWP(MN))*DDVI                 02190092
      DNEW=DEN(MN,I,J)                                                  02190093
      DOLD=DEN(MO,I,J)                                                  02190094
      DELT=DELT+TNEW*DDVI                                               02190095
      HNEW=HNEW+DHNEW*DDVI                                              02190096
      RNEW=RNEW+DNEW*DDVI                                               02190097
      COMP2=COMP2+DDVI                                                  02190098
80    CONTINUE                                                          02190099
      VOLOZU=VOLUP/DZ                                                   02190100
      VOLOZB=VOLBT/DZ                                                   02190101
      COMP2=COMP2+VOLOZU+VOLOZB                                         02190102
      SS   = SUPERS(TBOTT(MN),XSP(MN),XIP(MN),XWP(MN))                 02190103
      IF(SS.GT.SSMAX) SSMAX=SS                                          02190104
      IF(SS.LT.SSMIN) SSMIN=SS                                          02190105
      SUMG = SUMG+GROWTH(TBOTT(MN),SS,XIP(MN),XWP(MN))*VOLOZB           02190106
      SS   = SUPERS(TCALAV(MN),XSP(MN),XIP(MN),XWP(MN))                02190107
      IF(SS.GT.SSMAX) SSMAX=SS                                          02190108
      IF(SS.LT.SSMIN) SSMIN=SS                                          02190109
      SUMG = SUMG+GROWTH(TCALAV(MN),SS,XIP(MN),XWP(MN))*VOLOZU          02190110
```

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      DELT=DELT+VOLOZB*TBOTT(MN)                                                02190111
      RNEW=RNEW+VOLOZB*DBOTT(MN)                                                02190112
      HNEW=HNEW+VOLOZB*HBOTT(MN)                                                02190113
      DELT=DELT+VOLOZU*TCALAV(MN)                                               02190114
      RNEW=RNEW+VOLOZU*DCALAV(MN)                                               02190115
      HNEW=HNEW+VOLOZU*HCALAV(MN)                                               02190116
      DHNEW=PIE*DZ*HMAX*HMAX*HMAX*DENSTY*HNEW/BETA                              02190117
      TOTALH(MN)=DHNEW                                                          02190118
      DELT=DELT/COMP2                                                           02190119
      RNEW=RNEW/COMP2                                                           02190120
      AVERD(MN)=RNEW                                                            02190121
      AVERT(MN)=DELT                                                            02190122
C     AVERH(MN)=HNEW/RNEW/COMP2                                                 02190123
      AVERH(MN)=HNEW/COMP2                                                      02190124
          G(MN)=SUMG/COMP2                                                      02190125
      DELT=DELT-AVERT(MO)                                                       02190126
C                                                                               02190127
C     CALCULATION OF EVAPORATION RATE                                           02190128
C                                                                               02190129
      QQ=AQFLUX*AREAT/BETA*DENSTY                                               02190130
      C(MN)=QQ                                                                  02190131
      E(MN)=0.0                                                                 02190132
      DHOLD=TOTALH(MO)                                                          02190133
      DELH=((AVERH(MN)-AVERH(MO))*(HH(MO)+VOLC/RADSQ)*AVERD(MO)                 02190134
     1+(HH(MO)*AVERD(MO)-HH(MN)*AVERD(MN))*AVERH(MO))*RADSQ*DENSTY/BETA         02190135
      DELHV=(QQ+HF*F)*DT-DELH                                                   02190136
C*************************************************                          02190137
C***     THIS IS REALLY AN ERROR TEST     ************                         02190138
C*************************************************                          02190139
      E(MN)=DELHV/DT*BETA/HVAP                                                  02190140
C*********************************************************                  02190141
C*********************************************************                  02190142
      IF(E(MN).LT.0)  E(MN)=0.0                                                 02190143
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      EVINTO=E(MN)*DT+EVINTO                                          02190144
C*****************************************************************   02190145
      RETURN                                                          02190146
      END                                                             02190147
```

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      BLOCK DATA                                                        02190150
      IMPLICIT REAL*8(A-H,O-Z)                                          02190151
      REAL*8 IMP(2)                                                     02190152
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                 02190153
      DIMENSION ZPARS(5),ZPARV(4),ZPARH(8),ZPARG(9),ZPART(3)            02190154
      DIMENSION ZPARCP(4),ZPARBP(2),ZRATIO(3)                           02190155
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         02190156
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFIUX               02190157
      COMMON/REAL/ RTIME, TCONST                                        02190158
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02190159
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                02190160
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          02190161
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190162
      COMMON/STEP/MN,MO,N                                               02190163
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT       02190164
     1,DDDZDT(30,30),DDCDT(10)                                          02190165
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO         02190166
      COMMON/FORCE/ PUMPDP                                              02190167
      COMMON/INOUT/IN,IOUT                                              02190168
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190169
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190170
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190171
     3,          SSMAX, SSMIN                                          02190172
      COMMON/FLAG/ IWSTRT, IFLAG1, IFIAG2                               02190173
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      02190174
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190175
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190176
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190177
     3,          DZODTO                                                02190178
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02190179
     1,           FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                  02190180
     2,           HVINV,DELHLV,DENSTY                                  02190181
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190182
     1,           NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1               02190183
      COMMON/SIZE/H,RAD,HMAX                                            02190184
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190185
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1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                  02190186
2,NCALP1                                                                 02190187
 COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                    02190188
1,IDWNP1,IDOWM1                                                          02190189
 COMMON/AVPART/AVERNN(2),AVERLL(2)                                       02190190
 COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                         02190191
1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                      02190192
 COMMON/ENTLIM/XVLIM                                                     02190193
 COMMON/VAPDEN/PRESRF,RHOVR                                              02190194
 COMMON/ EMPEQ/ SLIPV, EXPV                                              02190195
 COMMON/ ITTER/ NSITER                                                   02190196
 COMMON/ EQUTON / RATCR                                                  02190197
 COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                    02190198
1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                                   02190199
2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)              02190200
3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                                02190201
 COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)              02190202
1,CALP(10,2)                                                             02190203
 COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                                 02190204
1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                        02190205
 COMMON / NMIJ/ N1, N2, N3                                               02190206
 COMMON / PARS/   PARS1, PARS2, PARS3, PARS4, PARS5                      02190207
 COMMON / PARV/ PARV1, PARV2, PARV3, PARV4                               02190208
 COMMON / PARH/  PARH1, PARH2, PARH3, PARH4,                             02190209
&               PARH5, PARH6, PARH7, PARH8                               02190210
 COMMON / PARG/ PARG1, PARG2, PARG3, PARG4,                              02190211
&              PARG5, PARG6, PARG7, PARG8, PARG9                         02190212
 COMMON / PART/ PART1, PART2, PART3                                      02190213
 COMMON / PRATIO/ PARR1, PARR2, PARR3                                    02190214
 COMMON / PARCP/ PRCP1, PRCP2, PRCP3, PRCP4                              02190215
 COMMON / PARBP/ PRBP1, PRBP2                                            02190216
 EQUIVALENCE (ZZZZ,WDWNJP)                                               02190217
 EQUIVALENCE (ZZZC,CALW)                                                 02190218
 EQUIVALENCE (ZPARS,PARS1)                                               02190219
 EQUIVALENCE (ZPARV,PARV1)                                               02190220
 EQUIVALENCE (ZPARH,PARH1)                                               02190221
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      EQUIVALENCE (ZPARG,PARG1)                                          02190222
      EQUIVALENCE (ZPART,PART1)                                          02190223
      EQUIVALENCE (ZPARCP,PRCP1)                                         02190224
      EQUIVALENCE (ZPARBP,PRBP1)                                         02190225
      EQUIVALENCE (ZRATIO,PARR1)                                         02190226
      DATA     PARR1/8.959873D0/, PARR2/0.15D0/, PARR3/0.0D0/            02190227
      DATA     PRCP1/1.0D0/, PRCP2/-0.1D0/, PRCP3/6.0D0/, PRCP4/0.6D0/   02190228
      DATA     PRBP1/2.2D0/, PRBP2/1.1D0/                                02190229
      DATA     PARS1/63.8188D0/, PARS2/-5.1082D-3/, PARS3/7.8360D-4/,     02190230
     &         PARS4/-1.5492D-6/, PARS5/0.083D0/                         02190231
      DATA     PARV1/10195.02D0/, PARV2/460.0D0/, PARV3/18.860D0/,       02190232
     &         PARV4/-26.523D0/                                          02190233
      DATA    PARH1/1075.84D0/, PARH2/0.434659D0/, PARH3/1.4877D-5/,     02190234
     &        PARH4/-7.0548D-7/, PARH5/3.756599D-3/, PARH6/0.44973521D0/,02190235
     &        PARH7/-6.9478D-5/, PARH8/-6.959D-6/                        02190236
      DATA     PARG1/11.0D0/, PARG2/-0.011D0/, PARG3/-140.0D0/,          02190237
     &         PARG4/8.0D0/, PARG5/0.004577D0/, PARG6/1.8D0/,            02190238
     &         PARG7/460.0D0/, PARG8/333.0D0/, PARG9/1.75D0/             02190239
      DATA     PART1/3061.596D0/, PART2/6.306699D0/, PART3/-383.7148D0/  02190240
      DATA RAD/ 6.0D0/,PRECMX/0.90D0/,WVOL/1200.0D0/, WHEIG/7.0D0/,      02190241
     1     AHTOV/1.50D0/, TUBEH/4.0D0/, TUBED/5.0D0/,                    02190242
     2     IMAX/12/, JJMAX/15/, IDOWN/6/,                                02190243
     3     ILEFT/8/, IRIGHT/12/, NCAL/5/                                 02190244
      DATA BETA/0.277D-3/, DELDDB/0.4635D0/, BRIXR/0.8D0/,               02190245
     1     RHOVR/0.576D-2/, DENSTY/88.1088D0/, TZERO/126.069D0/,         02190246
     2     HV/1127.3D0/, DELHLV/1006.38D0/, HR/94.03D0/                  02190247
      DATA F/0.00D+0/, BRIXFF/0.0D0/, PUFF/0.9D0/,                       02190248
     1     TSTEAM/280.0D0/, UU/90.0D0/, PRESRF/2.0D0/,                   02190249
     2     TEMPFF/105.0D0/                                               02190250
      DATA XSP/2*0.576D0/, XIP/2*0.064D0/, XCP/2*0.2D0/,                 02190251
     1     XWP/2*0.16D0/, AVERNN/2*0.1D+13/, AVERLL/2*3.281D-4/,         02190252
     2     RATCR/0.00D0/, TINTAL/134.979D0/                              02190253
      DATA NSITER/5/, SFSMTH/2.0D0/, THETAZ/0.5D0/,THETAS/0.75D0/,       02190254
     1     XVLIM/0.99999D0/, SLIPV/ 30.0D0/, EXPV/ 0.0D0/,               02190255
     2     PUMPDP/0.0D0/, VART/0.0D0/,ALPHA/1.339D-6/,                   02190256
     3     IWSTRT/1/, DT/0.1D-1/,                                        02190257
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3      N1/2/, N2/30/, N3/30/                                                  02190258
 DATA MN/1/, MO/2/, N/0/, JMAX/0/,                                            02190259
1      RTIME/0.0D0/, BTDUDT/0.0D0/, BTDEDT/0.0D0/,                            02190260
2      DDZDT/0.0D0/, SURFDT/0.0D0/, EVINTC/0.0D0/,                            02190261
3      EMVINT/0.0D0/, IFLAG1/0/, IFLAG2/0/                                    02190262
 DATA S/2*-0.9D+27/, C/2*-0.9D+27/, IMP/2*-0.9D+27/,                          02190263
1      EM/2*-0.9D+27/, Q/2*-0.9D+27/, AVERT/2*-0.9D+27/,                      02190264
2      AVERH/2*-0.9D+27/, AVERD/2*-0.9D+27/, TOTALH/2*-0.9D+27/               02190265
 DATA ZZZZ/40*-0.9D+27/, ZZZC/100*-0.9D+27/                                   02190266
      END                                                                     02190267
```

```
      SUBROUTINE BOUNDY                                                  02190270
C-----                                                                   02190271
C-----  SETS UP BOUNDARY CONDITIONS BETWEEN                              02190272
C-----  PAN PROPER AND THE LOWER PART OF PAN                             02190273
C-----  I.E. DOWNTAKE AND CALANDRIA.                                     02190274
C-----                                                                   02190275
      IMPLICIT REAL*8(A-H,O-Z)                                           02190276
      REAL*8 IMP(2)                                                      02190277
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)        02190278
     1,F,XWP,XSF,XIP,G(2),HF,AVERD(2),TMASS(2),WATER(2)                  02190279
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                    02190280
     3,            SSMAX, SSMIN                                         02190281
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX                02190282
      COMMON/FLAG/ IWSTRT, IFLAG1, IFLAG2                                02190283
      COMMON/REAL/ RTIME, TCONST                                         02190284
      COMMON/PAN/ VOLSCH, RADSQ, VCIC, WVCL, WHEIG                       02190285
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)            02190286
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                 02190287
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                           02190288
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ       02190289
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                    02190290
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                   02190291
     3,            DZODTO                                               02190292
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA               02190293
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 02190294
     2,             HVINV,DELHLV,DENSTY                                 02190295
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                           02190296
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT    02190297
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1              02190298
      COMMON/STEP/MN,MO,N                                                02190299
      COMMON/SIZE/H,RAD,HMAX                                             02190300
      COMMON /AREAP/DV(30),DVOA(30)                                      02190301
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                  02190302
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN               02190303
     1,IDWNP1,IDOWM1                                                    02190304
```

```
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH    02190305
     1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1            02190306
     2,NCALP1                                                           02190307
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)              02190308
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                             02190309
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)        02190310
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                          02190311
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)        02190312
     1,CALP(10,2)                                                       02190313
      COMMON/ CONECT/ HBNDS(30),DBNDS(30),TBNDS(30),QJCAL               02190314
      COMMON/ EMPEQ/ SLIPV, EXPV                                        02190315
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         02190316
      COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                02190317
     1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8              02190318
     1,              ENTHFR, FFLUXU                                     02190319
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/         02190320
      QJ=0.0                                                            02190321
      TJM1=CALT(NCAL,MC)                                                02190322
      DJM1=CALD(NCAL,MC)                                                02190323
      DO 391 I=ILEFT,IRIGHT                                             02190324
391   QJ=QJ+DV(I)*(T(MO,I,1)-TJM1)*(DEN(MO,I,1)*DZ+DJM1*CDZ)            02190325
      QJCAL=QJ/AFLWU/(DZ+CDZ)                                           02190326
      COMP11=0.0                                                        02190327
      HJJP1=0.0                                                         02190328
      DJJP1=0.0                                                         02190329
      TJJP1=0.0                                                         02190330
      DO 12 I=2,IDOWN                                                   02190331
      DDVI=DV(I)                                                        02190332
      HJJP1=HJJP1+DDVI*ENTH(MN,I,1)                                     02190333
      TJJP1=TJJP1+DDVI*T(MN,I,1)                                        02190334
      DJJP1=DJJP1+DDVI*DEN(MN,I,1)                                      02190335
      COMP11=COMP11+DDVI                                                02190336
12    CONTINUE                                                          02190337
```

```
      DHJP1=HJJP1/COMP11                                          02190338
      DJP1=DJJP1/COMP11                                           02190339
      TJP1=TJJP1/COMP11                                           02190340
      TDWNJP(MN)=TJP1                                             02190341
      DDWNJP(MN)=DJP1                                             02190342
      HDWNJP(MN)=DHJP1                                            02190343
      WJD=WDWNJP(MN)                                              02190344
      DO 2227 I=2,IDOWN                                           02190345
      HBNDS(I)=HBOTT(MN)                                          02190346
      DBNDS(I)=DBOTT(MN)                                          02190347
      TBNDS(I)=T(MN,I,1)                                          02190348
      WW(I,1)=WJD                                                 02190349
 2227 CONTINUE                                                    02190350
      DO 2228 I=IDWNP1,ILEFM1                                     02190351
      HBNDS(I)=ENTH(MN,I,1)                                       02190352
      DBNDS(I)=DEN(MN,I,1)                                        02190353
      TBNDS(I)=T(MN,I,1)                                          02190354
 2228 CONTINUE                                                    02190355
      DO 2230 I=IRIGP1,IMAX                                       02190356
      HBNDS(I)=ENTH(MN,I,1)                                       02190357
      DBNDS(I)=DEN(MN,I,1)                                        02190358
      TBNDS(I)=T(MN,I,1)                                          02190359
 2230 CONTINUE                                                    02190360
      HJM1=CALH(NCAL,MN)                                          02190361
      DJM1=CALD(NCAL,MN)                                          02190362
      TJM1=CALT(NCAL,MN)                                          02190363
      WJM1=CALH(NCAL,MN)/FMOM                                     02190364
      DO 2229 I=ILEFT,IRIGHT                                      02190365
      HBNDS(I)=HJM1                                               02190366
      DBNDS(I)=DJM1                                               02190367
      TBNDS(I)=T(MN,I,1)                                          02190368
      WW(I,1)=WJM1                                                02190369
 2229 CONTINUE                                                    02190370
      RETURN                                                      02190371
      END                                                         02190372
```

```
      SUBROUTINE CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                    02190375
C----                                                                    02190376
C----  CALCULATES MIXTURE DENSITY GIVEN ENTHALPY                         02190377
C----  AND PRESSURE, CORRECTS FOR PRESENCES OF                           02190378
C----  CRYSTALS.                                                         02190379
C----                                                                    02190380
      IMPLICIT REAL*8(A-H,O-Z)                                           02190381
      COMMON/VAPDEN/PRESRF,RHOVR                                         02190382
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA               02190383
     1,             FOURMF,FMO2DR,FMODR,CP,FOURMC,TZERO                 02190384
     2,             HVINV,DELHLV,DENSTY                                 02190385
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO          02190386
      TNEW=DHNEW/CP                                                      02190387
      TTSAT=TSAT(PJ)                                                     02190388
      TBOIL=TTSAT+BPE                                                    02190389
      IF(TNEW.LT.TBOIL) GO TO 99                                         02190390
      TNEW=TBOIL                                                         02190391
      HL=CP*TBOIL                                                        02190392
      RHOL=1.0D0-TNEW+DELRH                                              02190393
      RHOL=CONST1/RHOL+CONST2                                            02190394
      RHOL=1.0D0/RHOL                                                    02190395
      RHOV=RHOVR*(1.0D0+PJ/PRESRF)                                       02190396
      DELHLV=ENTHV(TTSAT,PJ,BPE)-HL                                      02190397
      XV=DHNEW/DELHLV-HL/DELHLV                                          02190398
      IF(XV.LT.XVLIM) GO TO 1                                            02190399
      DHNEW=HL+DELHLV*XVLIM                                              02190400
      XV=XVLIM                                                           02190401
 1    CONTINUE                                                           02190402
      XL=1.0D0-XV                                                        02190403
      DD=XL/RHOL+XV/RHOV                                                 02190404
      DD=1.0D0/DD                                                        02190405
      RETURN                                                             02190406
 99   XV=0.0                                                             02190407
      XL=1.0D0                                                           02190408
      DD=1.0D0-TNEW+DELRH                                                02190409
```

```
      DD=CONST1/DD+CONST2                                          02190410
      DD=1.0D0/DD                                                  02190411
      RETURN                                                       02190412
      END                                                          02190413
```

```
      SUBROUTINE CALHTD                                                      02190416
C-----                                                                       02190417
C-----  CALCULATES ENTHALPY AND TEMPERATURE FOR CALANDRIA                    02190418
C-----                                                                       02190419
      IMPLICIT REAL*8(A-H,O-Z)                                               02190420
      REAL*8 IMP(2)                                                          02190421
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5), QFLUX(10)                           02190422
      COMMON/ CONECT/ HBNDS(30),DBNDS(30),TBNDS(30),QJCAL                    02190423
      COMMON/ OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX                   02190424
      COMMON/ENTLIM/XVLIM                                                    02190425
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT            02190426
     1,DDDZDT(30,30),DDCDT(10)                                               02190427
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                   02190428
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                                  02190429
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)             02190430
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                               02190431
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)            02190432
     1,F,XWP,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                      02190433
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                        02190434
     3,             SSMAX, SSMIN                                            02190435
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                           02190436
      COMMON/PROPTY/RHC,RHOINV,RHOC2,VISC,ALPHA,VORHO,BETA                   02190437
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                     02190438
     2,             HVINV,DELHLV,DENSTY                                     02190439
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                               02190440
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT        02190441
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1                  02190442
      COMMON/STEP/MN,MO,N                                                    02190443
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)             02190444
     1,CALP(10,2)                                                            02190445
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTOLZ,DZODR,DZO2DR,DTO2DR,DTO2DZ           02190446
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                        02190447
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                       02190448
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     3,              DZCDTO                                                    02190449-
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH          02190450
     1,BOTTH,TUBED,PMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                  02190451
     2,NCALP1                                                                 02190452
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                       02190453
      COMMON/VAPDEN/PRESRF,RHOVR                                              02190454
      EQUIVALENCE (ZZZZ,WDWNJP)                                               02190455
      EQUIVALENCE (ZZZC,CALW)                                                 02190456
C                                                                             02190457
C      USE TO CHANGE HEAT LOAD (BY SPECIFYING CONSTANT QFLUX                  02190458
C      ,CHANGING TSTEAM, OR CALCULATING HEAT TRANSFER COEFF.)                 02190459
C                                                                             02190460
      CALL HEATIN( CALT, QFLUX, AQFLUX )                                      02190461
C                                                                             02190462
      SSUMT=0.0                                                               02190463
      SSUMH=0.0                                                               02190464
      SSUMD=0.0                                                               02190465
      QJ=QJCAL/CALPC2*CDZ                                                     02190466
      CALT(1,MO)=CALT(2,MO)                                                   02190467
      DJM1=CALD(NCAL,MO)                                                      02190468
      DO 2 JJ=1,NCALM1                                                        02190469
      J=NCAL-JJ                                                               02190470
      JP1=J+1                                                                 02190471
      DHOLD=CALH(JP1,MO)                                                      02190472
      TOLD=CALT(JP1,MO)                                                       02190473
      DOLD=DJM1                                                               02190474
      DJM1=CALD(J,MO)                                                         02190475
      QJP1=QJ                                                                 02190476
      QJ=(TOLD-CALT(J,MO))*(DJM1+DOLD)*0.5D0                                  02190477
      HCODT=(QFLUX(JP1)*POA-(DHOLD-CALH(J,MO))/CDZ                            02190478
     1*CALW(J,MO)*DJM1+(QJP1-QJ)*PCURMC/DT)/DOLD                              02190479
      DHNEW=DHOLD+HCODT*DT                                                    02190480
      HCDT(JP1)=HCODT                                                         02190481
C-------------------------------------------------                            02190482
C------ PRESSURE NOT ON STANDARD GRID INCREMENT ---                           02190483
      PJ=CALP(J,MO)                                                           02190484
```

```
C-------------------------------------------------------------      02190485
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                     02190486
      CALH(JP1,MN)=DHNEW                                            02190487
      CALD(JP1,MN)=DD                                               02190488
      CALT(JP1,MN)=TNEW                                             02190489
      SSUMT=SSUMT+TNEW                                              02190490
      SSUMD=SSUMD+DD                                                02190491
      SSUMH=SSUMH+DHNEW                                             02190492
 2    CONTINUE                                                      02190493
      COMP1=DFLOAT(NCALM1)                                          02190494
      TCALAV(MN)=SSUMT/COMP1                                        02190495
      HCALAV(MN)=SSUMH/COMP1                                        02190496
      DCALAV(MN)=SSUMD/COMP1                                        02190497
      RETURN                                                        02190498
      END                                                           02190499
```

```
      SUBROUTINE CALPP(PBIP1)                                                  02190502
C-----                                                                         02190503
C----  CALCULATES PRESSURE PROFILE IN CALANDRIA                                02190504
C-----                                                                         02190505
      IMPLICIT REAL*8(A-H,O-Z)                                                 02190506
      REAL*8 IMP(2)                                                            02190507
      DIMENSION ZZZC(10,2,5)                                                   02190508
      COMMON/LUMBT/ WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                    02190509
     1,             WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                      02190510
     2,             UBOTT(2),UCNEB(2),WCALAV(2),TCALAV(2),DCALAV(2)           02190511
     3,             HCALAV(2),WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)         02190512
      COMMON/CONC  /DELDDR,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO                02190513
      COMMON/PROPTY/ RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA                    02190514
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                       02190515
     2,              HVINV,DELHLV,DENSTY                                       02190516
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)              02190517
     1,           F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)            02190518
     2,           TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)              02190519
     3,           SSMAX, SSMIN                                                02190520
      COMMON/STEP/MN,MC,N                                                      02190521
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)               02190522
     1,CALP(10,2)                                                              02190523
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH          02190524
     1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                   02190525
     2,NCALP1                                                                  02190526
      EQUIVALENCE (ZZZC,CALW)                                                  02190527
C                                                                              02190528
      DPFRP= 8.0D0/TUBED/TUBED*VRATIO/DBOTT(MN)                                02190529
      BB   = (XIP(MN) + XSP(MN))/CONST1                                        02190530
      PJ=CALP(NCAL,MN)                                                         02190531
      DPDCJ  = 0.0                                                             02190532
      DO 2 JJ=1,NCALM1                                                         02190533
       J      = NCAL-JJ                                                       02190534
       JP1    = J + 1                                                         02190535
```

```
C------- PRESSURE IS OFF THE STANDARD GRID INCREMENT ----                02190536
C------- BECAUSE CALP(NCAL,MN) IS PRESS. AT TOP OF   ----                02190537
C------- CALANDRIA INSTEAD OF GRID POINT ABOVE THE CAL. -                02190538
        DPDCJP = DPDCJ                                                  02190539
        DJ     = CALD(JP1,MN)                                           02190540
        DPDCJ  = DPREF*VISCTY( CALT(JP1,MN) , BB )*(CALW(JP1,MN)*DJ      02190541
     &     +     CALW(JP1,MO)*CALD(JP1,MO)) + DJ                        02190542
        PJ     = PJ+(DPDCJP+DPDCJ)*CDZ*0.5D0                            02190543
 2      CALP(J,MN)=PJ                                                   02190544
C---------------------------------------------                          02190545
C------ PRESSURE FOR BOTTOM MOMENTUM BALANCE ---                        02190546
        PBIP1  =  PJ + DPDCJ*0.5D0*CDZ                                  02190547
C---------------------------------------------                          02190548
      RETURN                                                            02190549
      END                                                               02190550
```

```
      SUBROUTINE CALVAP                                                 02190553
C-----                                                                  02190554
C-----  CALCULATES MASS FLUX OF VAPOR                                   02190555
C----- LEAVING FREE SURFACE.                                           02190556
C-----                                                                  02190557
      IMPLICIT REAL*8(A-H,O-Z)                                          02190558
      REAL*8 IMP(2)                                                     02190559
      COMMON/CVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               02190560
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190561
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190562
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190563
     3,            SSMAX, SSMIN                                        02190564
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      02190565
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190566
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190567
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190568
     3,            DZODTO                                              02190569
      COMMON/PROPTY/RHO,RHOINV,RHOG2,VISC,ALPHA,VORHO,BETA              02190570
     1,            FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 02190571
     2,            HVINV,DELHLV,DENSTY                                 02190572
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190573
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190574
     1,            NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1              02190575
      COMMON/STEP/MN,MG,N                                               02190576
      COMMON/SIZE/H,RAD,HMAX                                            02190577
      COMMON /AREAP/DV(30),DVOA(30)                                     02190578
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                   02190579
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)               02190580
      COMMON/VAPDEN/PRESRF,RHOVR                                        02190581
      COMMON/ EMPEQ/ SLIPV, EXPV                                        02190582
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/         02190583
      COMP1=0.0                                                         02190584
      DO 32 I=2,IMAX                                                    02190585
      COMP2=RHOVR*SLIPV*SVFRV(I)*(1.0D0-SVFRV(I))**EXPV                 02190586
      COMP1=COMP1+DV(I)*COMP2                                           02190587
```

```
      FRAT(I)=CCMP2                                                    02190588
82    CONTINUE                                                         02190589
      EM(MN)=COMP1*DENSTY*HMAX**3*PIE                                  02190590
      EMVINT=EM(MN)*DT+EMVINT                                          02190591
      RETURN                                                           02190592
      END                                                              02190593
```

```
      SUBROUTINE CALWW                                                  02190596
C-----                                                                  02190597
C-----  CALCULATES MASS FLUX OF VAPOR LEAVING                           02190598
C-----  ONE-D CELL IN CALANDRIA, AND VELOCITY OF                        02190599
C-----  CELL CENTER.                                                    02190600
C-----                                                                  02190601
      IMPLICIT REAL*8(A-H,C-Z)                                          02190602
      REAL*8 IMP(2)                                                     02190603
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                 02190604
      COMMON/GRID/ DP,DZ,DT,DTCZSQ,DTODZ,DZODR,DZO2DP,DTO2DR,DTO2DZ     02190605
     1,            DT2DRZ,DTOLRZ,DTODR,FOURMD,DZOPSQ,DZODT,DTORSQ      02190606
     2,            DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DFT2,DZO,DDZDTO     02190607
     3,            DZODTO                                              02190608
      COMMON/PROPTY/ RHO,RHOINV,RHOC2,VISC,ALPHA,VORHO,BETA             02190609
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190610
     2,              HVINV,DELHLV,DENSTY                                02190611
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),ETLUDT,BTDEDT       02190612
     1,DDDZDT(30,30),DDCDT(10)                                          02190613
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)              02190614
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                             02190615
     2,UBOTT(2),UONER(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)        02190616
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                          02190617
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190618
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190619
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190620
     3,            SSMAX, SSMIN                                        02190621
      COMMON/STEP/MN,MC,N                                               02190622
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)        02190623
     1,CALP(10,2)                                                       02190624
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190625
     1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1            02190626
     2,NCALP1                                                           02190627
      EQUIVALENCE (ZZZZ,WDWNJP)                                         02190628
      EQUIVALENCE (ZZZC,CALW)                                           02190629
C                                                                       02190630
      SSUMW      = 0.0                                                  02190631
```

```
      RRWNEW      = WCALJM(MN)*DBOTT(MN)*FNOM                        02190632
      CALF(1,MN)  = RRWNEW/CALD(1,MN)                                02190633
      DO 1 J=2,NCAL                                                  02190634
      DD=CALD(J,MN)                                                  02190635
      RRWNEW=RRWNEW-CDZ*(DD-CALD(J,MO))/DT                           02190636
      WNEW=RRWNEW/DD                                                 02190637
      SSUMW=SSUMW+WNEW                                               02190638
      CALW(J,MN)=WNEW                                                02190639
1     CONTINUE                                                       02190640
      COMP1=DFLOAT(NCALM1)                                           02190641
      WCALAV(MN)=SSUMW/COMP1                                         02190642
      RETURN                                                         02190643
      END                                                            02190644
```

```
      SUBROUTINE CONTIN                                                 02190647
C-----                                                                  02190648
C-----  CALCULATES VERTICAL MASS FLUX LEAVING CELL                      02190649
C-----  IN PAN PROPER, AND THE VELOCITY OF EACH CELL                    02190650
C-----  CENTER.                                                         02190651
C-----                                                                  02190652
      IMPLICIT REAL*8(A-H,O-Z)                                          02190653
      REAL*8 IMP(2)                                                     02190654
      COMMON/MOVE    / DPDT(30)                                         02190655
      COMMON/ CONECT/ HBNDS(30),DBNDS(30),TBNDS(30),OJCAL               02190656
      COMMON/INOUT/IN,IOUT                                              02190657
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02190658
      COMMON/IPHASE/ENTH(2,30,30),DEN(2,30,30)                          02190659
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190660
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190661
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190662
     3,             DZODTO                                             02190663
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02190664
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190665
     2,             HVINV,DELHLV,DENSTY                                02190666
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190667
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190668
     1,             NPAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             02190669
      COMMON/STEP/MN,MC,N                                               02190670
      COMMON/SIZE/B,RAD,HMAX                                            02190671
      COMMON /AREAP/DV(30),DVOA(30)                                     02190672
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN              02190673
     1,IDWNP1,IDOWM1                                                    02190674
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190675
     1,BOTTH,TUBED,PMOM,CDZ,DTOCDZ,ISTEAM,NTUBES,NCAL,NCALM1            02190676
     2,NCALP1                                                           02190677
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT       02190678
     1,DDDZDT(30,30),BDCDT(10)                                          02190679
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         02190680
```

```
C                                                                       02190681
      DO 34 I=2,IMAX                                                    02190682
      IP1=I+1                                                           02190683
      IM1=I-1                                                           02190684
      IF(I.EQ.2) IM1=I                                                  02190685
      IF(I.EQ.IMAX) IP1=IMAX                                            02190686
      RIP1=R(IP1)                                                       02190687
      RIM1=R(IM1)                                                       02190688
      DJ=DBNDS(I)                                                       02190689
      WWW=WW(I,1)                                                       02190690
      DO 34 J=1,JMAX                                                    02190691
      JP1=J+1                                                           02190692
      DJM1=DJ                                                           02190693
      DJ=DEN(MN,I,J)                                                    02190694
      DIP1=DEN(MN,IP1,J)                                                02190695
      DIM1=DEN(MN,IM1,J)                                                02190696
      COMP1=RIM1*DIM1*U(MN,IM1,J)-RIP1*DIP1*U(MN,IP1,J)                 02190697
C                                                                       02190698
      IF(I.EQ.2) COMP1=-RIP1*DIP1*U(MN,IP1,J)                           02190699
     1-R(I)*DJ*U(MN,I,J)                                                02190700
      IF(I.EQ.IMAX) COMP1=R(I)*DJ*U(MN,I,J)                             02190701
     1+RIM1*DIM1*U(MN,IM1,J)                                            02190702
C                                                                       02190703
      AVDMDT=(DZ*DJ-DZO*DEN(MO,I,J))/DJ/DT                              02190704
      COMP1=0.5D0*DZO2DR*RINV(I)*COMP1/DJ-AVDMDT*0.5D0                  02190705
      WWW=WWW*DJM1/DJ+CCMP1                                             02190706
      W(MN,I,J)=WWW+DPDT(J)                                             02190707
C                                                                       02190708
      WWW=WWW+COMP1                                                     02190709
      WW(I,JP1)=WWW                                                     02190710
 34   CONTINUE                                                          02190711
      RETURN                                                            02190712
      END                                                               02190713
```

```
      SUBROUTINE CONTRL                                                 02190716
C-----                                                                  02190717
C-----  IMPOSES CONTRAINTS ON CALCULATION,                              02190718
C-----  PREFORMS CONTROL CALCULATIONS.                                  02190719
C-----    PRESENT USE-  MAINTAIN TOTAL MASS CONSTANT.                   02190720
C---- FEED CONTAINS NO SUGAR AND MATCHS EVAPORATION RATE                02190721
C-----                                                                  02190722
      IMPLICIT REAL*8(A-I,O-Z)                                          02190723
      REAL*8 IMP(2)                                                     02190724
      COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                02190725
     1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8              02190726
     1,              ENTHFR, FFLUXU                                     02190727
      COMMON/PROPTY/RHO,RHOINV,RHOCO2,VISC,ALPHA,VORHO,BETA             02190728
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190729
     2,             HVINV,DELHLV,DENSTY                                02190730
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190731
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190732
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190733
     3,           SSMAX, SSMIN                                         02190734
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190735
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190736
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190737
     3,           DZODTO                                               02190738
      COMMON/STEP/MN, MO, N                                             02190739
      COMMON/SIZE/ H, RAD, HMAX                                         02190740
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      02190741
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190742
     1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1            02190743
     2,NCALP1                                                           02190744
      COMMON/ VAPDEN /  PRESRF,RHOVR                                    02190745
      COMMON/ AVPART /  AVERNN(2), AVERLL(2)                            02190746
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                           02190747
     1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                  02190748
      DATA RHOC, COEFFV, PIE / 99.1D0, 0.5236D0, 3.14159D0 /            02190749
C                                                                       02190750
C                                                                       02190751
```

```
 F       = EM(MN)                                                          02190752
 ENTHFR  = F/DENSTY/HMAX**3/VOLBT/PIE                                      02190753
 FFLUXU  = F/DENSTY/HMAX**3/AFLWU/PIE                                      02190754
RETURN                                                                     02190755
 ENTRY ECNTRL                                                              02190756
 AVERNN(MN) = XCP(MN)*TMASS(MN)/RHOC/AVERLL(MN)**3/COEFFV                  02190757
 AVERNN(MO) = AVERNN(MN)                                                   02190758
RETURN                                                                     02190759
END                                                                        02190760
```

```
      SUBROUTINE CONVSF                                                 02190763
C-----                                                                  02190764
C-----   TRILIAGONAL IMPLICIT CALCULATION TO                            02190765
C-----   LOCATE FREE SURFACE.                                           02190766
C-----                                                                  02190767
      IMPLICIT REAL*8(A-H,O-Z)                                          02190768
      REAL*8 IMP(2)                                                     02190769
      DIMENSION AA(30),CC(30),DD(30),EE(30),FF(30),WH(30)               02190770
      DIMENSION AF(30),CF(30),BB(30),DDD(30)                            02190771
      COMMON/ ITTER/ NSITER                                             02190772
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190773
     1,           DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZOLT,DTORSQ       02190774
     2,           DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO      02190775
     3,           DZODTO                                               02190776
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190777
     1,             NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             02190778
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02190779
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02190780
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02190781
     3,           SSMAX, SSMIN                                         02190782
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               02190783
      COMMON/REAL/ RTIME, TCONST                                        02190784
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, HVOL, WHEIG                      02190785
      COMMON/AVPART/AVERNN(2),AVERLL(2)                                 02190786
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02190787
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                02190788
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          02190789
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02190790
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190791
     2,             HVINV,DELHLV,DENSTY                                02190792
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190793
      COMMON/STEP/MN,MO,N                                               02190794
      COMMON/SIZE/H,RAD,HMAX                                            02190795
      COMMON /AREAP/DV(30),DVOA(30)                                     02190796
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFBV(30),HVAP                   02190797
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)               02190798
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      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH    02190799
     1,BOITH,TUBED,FMCM,CDZ,DTCCDZ,TSTEAM,NTUBES,NCAI,NCAIM1            02190800
     2,NCAIP1                                                           02190801
      DATA EE(1)/1.0D0/, FF(1)/0.0D0/                                   02190802
C                                                                       02190803
      DO   1   I=3,IMAXM1                                               02190804
      IM1     = I - 1                                                   02190805
      IP1     = I + 1                                                   02190806
      DDD(I)  =  WW(I,JMAXP1)*DEN(MN,I,JMAX)-FRAT(I)                    02190807
      DD(I)   =  DDD(I)*DT                                              02190808
     & +SURFAC(I)*DEN(MO,I,JMAXP1)                                      02190809
      AA(I)   = -R(IP1)*U(MN,IP1,JMAXP1) * RINV(I) * DTO2DR             02190810
     & + AF(I)                                                          02190811
 1    CC(I)   =  R(IM1)*U(MN,IM1,JMAXP1) * RINV(I) * DTO2DR             02190812
     & + CF(I)                                                          02190813
C-----  BOUNDRY CONDITIONS ----------------------------                02190814
      DDD(2)      = WW(2,JMAXP1)*DEN(MN,2,JMAX)-FRAT(2)                 02190815
      DD(2)       = DDD(2)*DT                                           02190816
     & +SURFAC(2)*DEN(MO,2,JMAXP1)                                      02190817
      AA(2)       = -R(3)*U(MN,3,JMAXP1) * RINV(2) * DTO2DR             02190818
     & + AF(2)                                                          02190819
      CC(2)       = -U(MN,2,JMAXP1) * DTO2DR                            02190820
     & + CF(2)                                                          02190821
      DDD(IMAX)   =  WW(IMAX,JMAXP1)*DEN(MN,IMAX,JMAX)-FRAT(IMAX)       02190822
      DD(IMAX)    =  DDD(IMAX)*DT                                       02190823
     & +SURFAC(IMAX)*DEN(MO,IMAX,JMAXP1)                                02190824
      AA(IMAX)    =  U(MN,IMAX,JMAXP1) * DTO2DR                         02190825
     & + AF(IMAX)                                                       02190826
      CC(IMAX)    =  R(IMAXM1)*U(MN,IMAXM1,JMAXP1)*RINV(IMAX)*DTO2DR    02190827
     & + CF(IMAX)                                                       02190828
C-------------------------------------------------------               02190829
      DO   2   I=2,IMAX                                                 02190830
      COMP1  = BB(I) - CC(I) * EE(I-1)                                  02190831
      EE(I)  = AA(I)/COMP1                                              02190832
 2    FF(I)  = (DD(I) + CC(I) * FF(I-1))/COMP1                          02190833
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```
      WH(IMAXP1)  = FF(IMAX)/(1.0D0 - EE(IMAX))                          02190834
      SMIN        = 1000.0                                               02190835
      SURFHN      = 0.0                                                  02190836
      RATZ        = DDZDT*DFLOAT(JMAX)                                   02190837
      DO    3    II=1,IMAXM1                                             02190838
      I           = IMAXP1 - II                                          02190839
      DNEW        = DEN(MN,I,JMAXP1)                                     02190840
      WH(I)       = EE(I) * WH(I+1) + FF(I)                              02190841
      SURFI       = WH(I)/DNEW                                           02190842
      SURFHN      = SURFHN+DVOA(I)*SURFI                                 02190843
      IF(SURFI.LT.SMIN) SMIN=SURFI                                       02190844
      RATH        = (SURFI-SURFAC(I))/DT                                 02190845
      W(MN,I,JMAXP2) = RATH + RATZ                                       02190846
      W(MN,I,JMAXP1) = 0.5D0*(RATH + DDD(I)/DNEW) + RATZ                 02190847
C     SSURF(I)    = SURFI                                                02190848
 3    SURFAC(I)   = SURFI                                                02190849
      WH(1)       = WH(2)                                                02190850
C---- DO    4    I=2,IMAX                                                02190851
C4--- DHDT(I)    =( ((AA(I)-AF(I))*WH(I+1)+(CC(I)-CF(I))*WH(I-1))/DT    02190852
C---  & + DDD(I) )/DEN(MN,I,JMAXP1)                                      02190853
C                                                                        02190854
      HH(MN)=(SURFHN+JMAX*DZ)*HMAX+CALANH                                02190855
      SMIN=SMIN-0.10D0*DZ                                                02190856
      IF(SMIN.GT.0.0) GO TO 50                                           02190857
      CALL OUTPUT                                                        02190858
      CALL CUTALL                                                        02190859
      STOP 50                                                            02190860
 50   CONTINUE                                                           02190861
      RETURN                                                             02190862
      ENTRY INCONV                                                       02190863
      DO    10    I=2,IMAXM1                                             02190864
      BB(I)       = 1.0D0  +  2.0D0*SFSMTH*DTORSQ                        02190865
      AF(I)       =  SFSMTH*DTORSQ*RH(I)*RINV(I)                         02190866
 10   CF(I)       =  SFSMTH*DTORSQ*RH(I-1)*RINV(I)                       02190867
      BB(2)       = 1.0D0  +      SFSMTH*DTORSQ*RH(2)*RINV(2)            02190868
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      AF(2)      =  SFSMTH*DTORSQ*RH(2)*RINV(2)                                  02190869
      CF(2)      =  0.0D0                                                        02190870
      BB(IMAX)   = 1.0D0  +      SFSMTH*DTORSQ*RH(IMAXM1)*RINV(IMAX)             02190871
      AF(IMAX)   =  0.0D0                                                        02190872
      CF(IMAX)   =  SFSMTH*DTORSQ*RH(IMAXM1)*RINV(IMAX)                          02190873
      RETURN                                                                     02190874
      END                                                                        02190875
```

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      SUBROUTINE ENERGY                                                 02190878
C-----                                                                  02190879
C-----  INTEGRATION OF ENERGY EQUATION                                  02190880
C-----                                                                  02190881
      IMPLICIT REAL*8(A-H,O-Z)                                          02190882
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         02190883
      COMMON /AREAP/DV(30),DVOA(30)                                     02190884
      COMMON/DIMEN/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02190885
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                02190886
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02190887
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02190888
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02190889
     3,             DZODTO                                             02190890
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02190891
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                02190892
     2,              HVINV,DELHLV,DENSTY                                02190893
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02190894
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02190895
     1,             NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             02190896
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN              02190897
     1,IDWNP1,IDOWM1                                                   02190898
      COMMON/STEP/MN,MO,N                                               02190899
      COMMON/SUBDER/DPDTI                                               02190900
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT       02190901
     1,DDDZDT(30,30),DDCDT(10)                                          02190902
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH   02190903
     1,BOTTH,TUBED,PMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1            02190904
     2,NCALP1                                                           02190905
      COMMON/TEMP/TNEW,TOLD,TIP1,TIM1,TJP1,TJM1                         02190906
      COMMON/CONSER/DIP1,DIM1,DJP1,DJM1,RIP1,RIM1,RI,RHIP1,RHIM1        02190907
     1,ADIP1,ADIM1,ADJP1,ADJM1                                          02190908
      COMMON/VELCTY/UNEW,UOLD,WNEW,WOLD,UIP1,UIM1,UJP1,UJM1,WIP1,WIM1   02190909
     1,WJP1,WJM1,UF,UB,WF,WB                                            02190910
      COMMON/INDEX/I,J                                                  02190911
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                 02190912
C                                                                       02190913
```

```
      HUF=0.0                                                                  02190914
      IF(UF.LT.0.0)  HUF=DHIP1-DHOLD                                           02190915
      HUB=DHIM1-DHOLD                                                          02190916
      IF(UB.LT.0.0)  HUB=0.0                                                   02190917
      HWF=0.0                                                                  02190918
      IF(WF.LT.0.0)  HWF=DHJP1-DHOLD                                           02190919
      HWB=DHJM1-DHOLD                                                          02190920
      IF(WB.LT.0.0)  HWB=0.0                                                   02190921
C                                                                              02190922
C                                                                              02190923
C                                                                              02190924
      COMP1=DTODZ*(WF*HWF-WB*HWB)                                              02190925
      COMP2=DTO2DR*RINV(I)*(UF*HUF-UB*HUB)                                     02190926
      CCMP3=FOURMD*((TJP1-TOLD)*ADJP1-(TOLD-TJM1)*ADJM1)                       02190927
      IF(J.EQ.1.AND.I.GT.ILEFM1)  COMP3=FOURMD*((TJP1-TOLD)*ADJP1              02190928
     1-(TOLD-TJM1)/FMCM/CALFC2*DZ*ADJM1)                                       02190929
      COMP4=FOURMR*RINV(I)*(RHIP1*(TIP1-TOLD)*ADIP1                            02190930
     1-RHIM1*(TOLD-TIM1)*ADIM1)                                                02190931
      DEODT=(-COMP1-COMP2+COMP3+COMP4)*RHOINV                                  02190932
      DHNEW=DHOLD+DEODT                                                        02190933
      DEDT(I,J)=DEODT/DT                                                       02190934
C---- QJ=FOURMD*DZODT*(TOLD-TJM1)*ADJM1                                        02190935
C---- IF(J.EQ.1.AND.I.GT.ILEFM1) QJ=ALPHA*ADJM1/FMOM*(TOLD-TJM1)/CALFC2        02190936


      RETURN                                                                   02190937
      END                                                                      02190938
                                                                               02190939
```

```
      REAL FUNCTION VISCTY*8(T,B)                                        02190941
C---- VISCOSITY                                                         02190942
      IMPLICIT REAL*8 (A-H,O-Z)                                          02190943
      COMMON / SPARV/ SPARV1, SPARV2, SPARV3, SPARV4                     02190944
      VISCTY=DEXP(SPARV1/(T+SPARV2)+SPARV3*B+SPARV4)                     02190945
      RETURN                                                             02190946
      END                                                                02190947
CCC                                                                      02190948
CCC                                                                      02190949
      REAL FUNCTION HEATC*8(XCP,B)                                       02190950
C---- HEAT CAPACITY                                                      02190951
      IMPLICIT REAL*8 (A-H,O-Z)                                          02190952
      COMMON / SPARCP/ SPRCP1, SPRCP2, SPRCP3, SPRCP4                    02190953
      HEATC = SPRCP1 + (SPRCP2 + SPRCP3*XCP)*B                           02190954
      RETURN                                                             02190955
      END                                                                02190956
CCC                                                                      02190957
CCC                                                                      02190958
      REAL FUNCTION BOILPE*8(XIP,XWP,B)                                  02190959
C---- BOILING POINT ELEVATION                                            02190960
      IMPLICIT REAL*8 (A-H,O-Z)                                          02190961
      COMMON / SPARBP/ SPRBP1, SPRBP2                                    02190962
      BOILPE = SPRBP1*(B/XWP)+SPRBP2*(XIP/B)                             02190963
      RETURN                                                             02190964
      END                                                                02190965
CCC                                                                      02190966
CCC                                                                      02190967
      REAL FUNCTION SUPERS*8(T,XSP,XIP,XWP)                              02190968
C---- SUPERSATURATION                                                    02190969
      IMPLICIT REAL*8 (A-H,O-Z)                                          02190970
      COMMON / SPARS/ SPARS1, SPARS2, SPARS3, SPARS4, SPARS5             02190971
      SAT=SPARS1 +(SPARS2 + SPARS3*T + SPARS4*T*T)*T                     02190972
      SUPERS=(100.0-SAT)/SAT*XSP/XWP*(1.0/(1.0-SPARS5*XIP/XWP))          02190973
      RETURN                                                             02190974
      END                                                                02190975
```

```
      REAL FUNCTION GROWTH*8(T,SS,XIP,XWP)                                  02190978
C----   GROWTH RATE                                                         02190979
      IMPLICIT REAL*8 (A-H,O-Z)                                             02190980
      COMMON / SPARG/ SPARG1, SPARG2, SPARG3, SPARG4,                       02190981
     &                SPARG5, SPARG6                                       02190982
      COMMON/ EQUTON / RATCR                                                02190983
      EACT=SPARG1 + SPARG2*T + SPARG3*XIP/XWP                               02190984
      RATC=RATCR*DEXP(-EACT*(1.0D0/(T+SPARG4)-SPARG5)+SPARG6*XIP/XWP)       02190985
      OS=SS-1.0                                                             02190986
      GROWTH=RATC*OS                                                        02190987
      IF(OS.LT.0.0) GROWTH=5.0*GROWTH                                       02190988
      RETURN                                                                02190989
      END                                                                   02190990
CCC                                                                         02190991
CCC                                                                         02190992
      REAL FUNCTION RATIO*8(V,X)                                            02190993
C----   EFFECT OF CRYSTALS ON VISCOSITY                                     02190994
      IMPLICIT REAL*8 (A-H,O-Z)                                             02190995
      COMMON / SPRATO/ SPARR1, SPARR2, SPARR3                               02190996
      RATIO = DEXP(SPARR1*V*X**SPARR2)                                      02190997
      RETURN                                                                02190998
      END                                                                   02190999
CCC                                                                         02191000
CCC                                                                         02191001
      REAL FUNCTION TSAT*8(PJ)                                              02191002
C----   BOILING POINT OF PURE WATER                                         02191003
      IMPLICIT REAL*8 (A-H,O-Z)                                             02191004
      COMMON/VAPDEN/PRESRF,RHOVR                                            02191005
      COMMON / SPART/ SPART1, SPART2, SPART3                                02191006
      TSAT=SPART1/(SPART2-DLOG10(PJ+PRESRF))+ SPART3                        02191007
      RETURN                                                                02191008
      END                                                                   02191009
```

```
      REAL FUNCTION ENTHV*8(TT,PP,DDT)                                  02191012
C-----    ENTHALPY OF VAPOR                                             02191013
      IMPLICIT REAL*8 (A-H,O-Z)                                         02191014
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                           02191015
     1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                 02191016
      COMMON / SPARH/ SPARH1, SPARH2, SPARH3, SPARH4,                   02191017
     &                SPARH5, SPARH6, SPARH7, SPARH8, SPARH9            02191018
      ENTHV= SPARH1  + (SPARH2 + SPARH3*TT + SPARH4*TT*TT)*TT           02191019
     1      +(PP*SPARH5 + SPARH6 + SPARH7*PP*PP                        02191020
     1      +SPARH8*DDT*PP + SPARH9*DDT )*DDT                          02191021
      RETURN                                                            02191022
      END                                                               02191023
CCC                                                                     02191024
CCC                                                                     02191025
      REAL FUNCTION VKINEM*8(TT,BB)                                     02191026
C-----      CALCULATE KINEMATIC VISCOSITY                               02191027
C-----     (VART IS ARTIFICIAL VISCOSITY = 0)                           02191028
      IMPLICIT REAL*8 (A-H,O-Z)                                         02191029
      REAL*8 IMP(2)                                                     02191030
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02191031
     1,            F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)    02191032
     2,            TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)      02191033
     3,            SSMAX, SSMIN                                        02191034
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                           02191035
     1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                 02191036
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO         02191037
      COMMON/STEP  /MN, MO, N                                           02191038
       VKINEM = VART  + VISCTY(TT,BB)*VRATIO/AVERD(MN)                  02191039
C      VKINEM = VART                                                    02191040
      RETURN                                                            02191041
      END                                                               02191042
---
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      SUBROUTINE HEATIN( CALT,  QFLUX, AQFLUX )                          02191045
C----  CALCULATES OR IMPOSES HEAT FLUX IN CALANDRIA                       02191046
      IMPLICIT REAL*8 (A-H,O-Z)                                          02191047
      DIMENSION CALT(10,2), QFLUX(10)                                    02191048
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                    02191049
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                02191050
      COMMON/REAL/ RTIME, TCONST                                         02191051
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA               02191052
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 02191053
     2,             HVINV,DELHLV,DENSTY                                 02191054
      COMMON/STEP/ MN, MO, N                                             02191055
      COMMON/SIZE/ H, RAD, HMAX                                          02191056
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH    02191057
     1,           BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1 02191058
     2,           NCALP1                                                02191059
        AQFLUX   = FLUX                                                  02191060
        DO  1   J = 2, NCAL                                              02191061
1       QFLUX(J)  = FLUX                                                 02191062
      RETURN                                                             02191063
        ENTRY INHEAT(EVAP)                                               02191064
C------  ENTER EVAPORATION COEFFICENT --------------                     02191065
        FLUX = EVAP*HVAP/3600.0*TCONST/DENSTY                            02191066
      RETURN                                                             02191067
      END                                                                02191068
```

```
      SUBROUTINE HUNEW                                                  02191071
C-----                                                                  02191072
C-----  SET UP FOR INTEGRATION OF ENERGY AND MOMENTUM EQUATIONS         02191073
C-----                                                                  02191074
      IMPLICIT REAL*8(A-H,O-Z)                                          02191075
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                 02191076
      REAL*8 IMP(2)                                                     02191077
      COMMON/ CONECT/ HBNDS(30),DBNDS(30),TBNDS(30),QJCAL               02191078
      COMMON/MOVE   / DPDT(30)                                          02191079
      COMMON/FORCE/ PUMPDP                                              02191080
      COMMON/INOUT/IN,IOUT                                              02191081
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       02191082
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 02191083
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   02191084
     3,          SSMAX, SSMIN                                          02191085
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               02191086
      COMMON/FLAG/ IWSTRT, IFLAG1, IFLAG2                               02191087
      COMMON/REAL/ RTIME, TCONST                                        02191088
      COMMON/PAM/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      02191089
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           02191090
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                02191091
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          02191092
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      02191093
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   02191094
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  02191095
     3,          DZODTO                                                02191096
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              02191097
     1,           FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                   02191098
     2,           HVINV,DELHLV,DENSTY                                   02191099
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          02191100
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   02191101
     1,           NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1                02191102
      COMMON/STEP/MN,MO,N                                               02191103
      COMMON/TEMP/TNEW,TOLD,TIP1,TIM1,TJP1,TJM1                         02191104
      COMMON/CONSER/DIP1,DIM1,DJP1,DJM1,RIP1,RIM1,RI,RHIP1,RHIM1        02191105
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     1,ADIP1,ADIM1,ADJP1,ADJM1                                                  02191106
      COMMON/VELCTY/UNEW,UOLD,WNEW,WOLD,UIP1,UIM1,UJP1,UJM1,WIP1,WIM1           02191107
     1,WJP1,WJM1,UF,UB,WF,WB                                                    02191108
      COMMON/PRESS/PIP1,PIM1,PJ,PJP1                                            02191109
      COMMON/SIZE/H,RAD,HMAX                                                    02191110
      COMMON/INDEX/I,J                                                          02191111
      COMMON /AREAP/DV(30),DVOA(30)                                             02191112
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                         02191113
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                      02191114
     1,IDWNP1,IDOWM1                                                            02191115
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH           02191116
     1,BOTTH,TUBED,FMCH,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                    02191117
     2,NCALP1                                                                   02191118
      COMMON /FLOW/DWT                                                          02191119
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT               02191120
     1,DDDZDT(30,30),DDCDT(10)                                                  02191121
      COMMON/AVPART/AVERNN(2),AVERLL(2)                                         02191122
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                           02191123
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                       02191124
      COMMON/SUBDER/DPDTI                                                       02191125
      COMMON/ENTLIM/XVLIM                                                       02191126
      COMMON/VAPDEN/PRESRF,RHOVR                                                02191127
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                      02191128
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                                     02191129
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)                02191130
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                                  02191131
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)                02191132
     1,CALP(10,2)                                                               02191133
      COMMON/ EMPEQ/ SLIPV, EXPV                                                02191134
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)                 02191135
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/                 02191136
      EQUIVALENCE (ZZZZ,WDWNJP)                                                 02191137
      EQUIVALENCE (ZZZC,CALW)                                                   02191138
C                                                                               02191139
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```
      DO 11 I=2,IMAX                                                    02191140
      IM1=I-1                                                           02191141
      IP1=I+1                                                           02191142
      IF(I.EQ.2) IM1=I                                                  02191143
      IF(I.EQ.IMAX) IP1=IMAX                                            02191144
      RIP1=R(IP1)                                                       02191145
      RIM1=R(IM1)                                                       02191146
      RI=R(I)                                                           02191147
      RHIP1=RH(I)                                                       02191148
      RHIM1=RH(IM1)                                                     02191149
      HI=SURFAC(I)                                                      02191150
      HIP1=SURFAC(IP1)                                                  02191151
      HIM1=SURFAC(IM1)                                                  02191152
      SURFI=(HI+DZ)*0.5D0                                               02191153
      PIM1=P(IM1,JMAXP1)                                                02191154
      PIP1=P(IP1,JMAXP1)                                                02191155
      PJ=P(I,JMAXP1)                                                    02191156
      UOLD=U(MO,I,JMAXP1)                                               02191157
      UJP1=UOLD                                                         02191158
      UJM1=U(MO,I,JMAX)                                                 02191159
      UIM1=U(MO,IM1,JMAXP1)                                             02191160
      UIP1=U(MO,IP1,JMAXP1)                                             02191161
      RHO=DEN(MO,I,JMAXP1)                                              02191162
      DJM1=DEN(MO,I,JMAX)                                               02191163
      DJP1=RHO                                                          02191164
      DIP1=DEN(MO,IP1,JMAXP1)                                           02191165
      DIM1=DEN(MO,IM1,JMAXP1)                                           02191166
      ADIP1=(DIP1+RHO)/2.0D0                                            02191167
      ADIM1=(RHO+DIM1)/2.0D0                                            02191168
      ADJM1=(RHO*HI+DJM1*DZ)/(HI+DZ)                                    02191169
      RHOINV=1.0D0/RHO                                                  02191170
      HHIP1=(HIP1+HI)/2.0D0                                             02191171
      HHIM1=(HIM1+HI)/2.0D0                                             02191172
      DTOHI=DT/HI                                                       02191173
```

```
      UF=RIP1*HIP1*DIP1*UIP1+RI*HI*RHO*UOLD                              02191175
      UB=RIM1*HIM1*DIM1*UIM1+RI*HI*RHO*UOLD                              02191176
      IF(I.EQ.2) UB=0.0                                                  02191177
      IF(I.EQ.IMAX) UF=0.0                                               02191178
      UUF=0.0                                                            02191179
      IF(UF.LT.0.0) UUF=UIP1-UOLD                                        02191180
      UUB=UIM1-UOLD                                                      02191181
      IF(UB.LT.0.0) UUB=0.0                                              02191182
      WB=WW(I,JMAXP1)*DJM1                                               02191183
      UWB=UJM1-UOLD                                                      02191184
      IF(WB.LT.0.0) UWB=0.0                                              02191185
C                                                                        02191186
CC                                                                       02191187
C                                                                        02191188
      COMP1=DTO2DR*RINV(I)*(UF*UUF-UB*UUB)/HI                            02191189
      COMP2=DTOHI*UWB*WB                                                 02191190
      COMP3=VORHO*DTOHSQ*RINV(I)*(RHIP1*(UIP1-UOLD)*HHIP1*ADIP1          02191191
     1-RHIM1*(UOLD-UIM1)*HHIM1*ADIM1)/HI                                 02191192
      COMP5=VORHO*DTOHI*(UJM1-UOLD)/SURFI*ADJM1                          02191193
      COMP6=DTO2DR*((PIM1+PJ)*HHIM1-(PIP1+PJ)*HHIP1)/HI                  02191194
      COMP7=-VORHO*DT*RINV(I)*RINV(I)*UOLD                               02191195
      DUODT=(-COMP1+COMP2+COMP3+COMP5+COMP6)*RHOINV+COMP7                02191196
      UNEW=UOLD+(DUDT(I,JMAXP1)*DT+DUODT)*0.5D0                          02191197
      DUDT(I,JMAXP1)=DUODT/DT                                            02191198
      U(MN,I,JMAXP1)=UNEW                                                02191199
C                                                                        02191200
      TJM1=T(MO,I,JMAX)                                                  02191201
      TOLD=T(MO,I,JMAXP1)                                                02191202
      TJP1=TOLD                                                          02191203
      TIP1=T(MO,IP1,JMAXP1)                                              02191204
      TIM1=T(MO,IM1,JMAXP1)                                              02191205
      DHJM1=ENTH(MO,I,JMAX)                                              02191206
      DHOLD=ENTH(MO,I,JMAXP1)                                            02191207
      DHJP1=DHOLD                                                        02191208
      DHIP1=ENTH(MO,IP1,JMAXP1)                                          02191209
      DHIM1=ENTH(MO,IM1,JMAXP1)                                          02191210
```

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C                                                                       02191211
      HUF=0.0                                                           02191212
      IF(UF.LT.0.0)  HUF=DHIP1-DHOLD                                    02191213
      HUB=DHIM1-DHOLD                                                   02191214
      IF(UB.LT.0.0)  HUB=0.0                                            02191215
      HWB=DHJM1-DHOLD                                                   02191216
      IF(WB.LT.0.0)  HWB=0.0                                            02191217
C                                                                       02191218
CC                                                                      02191219
C                                                                       02191220
      COMP1=DTO2DR*RINV(I)*(HUF*UF-HUB*UB)/HI                           02191221
      COMP2=DTOHI*(FRAT(I)*(HVAP-DHCLD)-WB*HWB)                         02191222
      COMP3=FOURHR*RINV(I)*(RHIP1*(TIP1-TOLD)*HHIP1*ADIP1               02191223
     1-RHIM1*(TOLD-TIM1)*HHIM1*ADIM1)/HI                                02191224
      COMP4=ALPHA*DTOHI*(TJM1-TOLD)/SURFI*ADJM1                         02191225
      DEODT=(-COMP1-CCMP2+COMP3+CCMP4)*RHOINV                           02191226
C     DHNEW=DHOLD+(DEDT(I,JMAXP1)*DT+DEODT)*0.5D0                       02191227
      DHNEW=DHOLD+DEODT                                                 02191228
      DEDT(I,JMAXP1)=DEODT/DT                                           02191229
C                                                                       02191230
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                         02191231
      ENTH(MN,I,JMAXP1)=DHNEW                                           02191232
      T(MN,I,JMAXP1)=TNEW                                               02191233
      DEN(MN,I,JMAXP1)=DD                                               02191234
C                                                                       02191235
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,0.0D0,0.999999D+00)               02191236
      SVFRV(I)=XV*DD/RHOVR                                              02191237
      T(MN,I,JMAXP2)=TNEW                                               02191238
      DEN(MN,I,JMAXP2)=DD                                               02191239
      ENTH(MN,I,JMAXP2)=DHNEW                                           02191240
C                                                                       02191241
```

```
C                                                                       02191242
C C                                                                     02191243
C                                                                       02191244
      TJP1=TOLD                                                         02191245
      TOLD=TJM1                                                         02191246
      UJP1=UOLD                                                         02191247
      UOLD=UJM1                                                         02191248
      DHJP1=DHOLD                                                       02191249
      DHOLD=DHJM1                                                       02191250
      DJP1=RHO                                                          02191251
      RHO=DJM1                                                          02191252
      UJM1=U(MO,I,JMAXM1)                                               02191253
      UIP1=U(MO,IP1,JMAX)                                               02191254
      UIM1=U(MO,IM1,JMAX)                                               02191255
      PIP1=P(IP1,JMAX)                                                  02191256
      PIM1=P(IM1,JMAX)                                                  02191257
      PJ=P(I,JMAX)                                                      02191258
      DIP1=DEN(MO,IP1.JMAX)                                             02191259
      DIM1=DEN(MO,IM1,JMAX)                                             02191260
      DJM1=DEN(MO,I,JMAXM1)                                             02191261
      ADIP1=(DIP1+RHO)/2.0D0                                            02191262
      ADIM1=(RHO+DIM1)/2.0D0                                            02191263
      ADJP1=ADJM1                                                       02191264
      ADJM1=(RHO+DJM1)/2.0D0                                            02191265
      RHOINV=1.0D0/RHO                                                  02191266
C                                                                       02191267
      UF=RIP1*DIP1*UIP1+RI*RHO*UOLD                                     02191268
      UB=RIM1*DIM1*UIM1+RI*RHO*UOLD                                     02191269
      IF(I.EQ.2) UB=0.0                                                 02191270
      IF(I.EQ.IMAX) UF=0.0                                              02191271
      UUF=0.0                                                           02191272
      IF(UF.LT.0.0) UUF=UIP1-UOLD                                       02191273
      UUB=UIM1-UOLD                                                     02191274
      IF(UB.LT.0.0) UUB=0.0                                             02191275
      WF=WB                                                             02191276
      WB=DJM1*WW(I,JMAX)                                                02191277
```

```
      UWF=0.0                                                                  02191278
      IF(WF.LT.0.0)  UWF=UJP1-UOLD                                             02191279
      UWB=UJM1-UOLD                                                            02191280
      IF(WB.LT.0.0)  UWB=0.0                                                   02191281
C                                                                              02191282
CC                                                                             02191283
C                                                                              02191284
      COMP1=DTO2DR*RINV(I)*(UUF*UF-UUB*UB)                                     02191285
      COMP2=DTODZ*(UWF*WF-UWB*WB)                                              02191286
      COMP3=VORHO*DTORSQ*RINV(I)*(RHIP1*(UIP1-UOLD)*AIP1                       02191287
     1-RHIM1*(UOLD-UIM1)*AIM1)                                                 02200000
      COMP5=VORHO*DTODZ*(ADJP1*(UJP1-UOLD)/SURFI-ADJM1*(UOLD-UJM1)/DZ)         02210000
      COMP6=DTO2DR*(PIM1-PIP1)                                                 02220000
      COMP7=-VORHO*RINV(I)*RINV(I)*UOLD*DT                                     02230000
      DUODT=(-COMP1-COMP2+COMP3+COMP5+COMP6)*RHOINV+COMP7                      02240000
      UNEW=UOLD+0.5D0*(DUDT(I,JMAX)*DT+DUODT)                                  02250000
      DUDT(I,JMAX)=DUODT/DT                                                    02260000
      U(MM,I,JMAX)=UNEW                                                        02270000
C                                                                              02280000
      DHJM1=ENTH(MO,I,JMAXM1)                                                  02290000
      DHIP1=ENTH(MO,IP1,JMAX)                                                  02300000
      DHIM1=ENTH(MO,IM1,JMAX)                                                  02310000
      TIP1=T(MO,IP1,JMAX)                                                      02320000
      TIM1=T(MO,IM1,JMAX)                                                      02330000
      TJM1=T(MO,I,JMAXM1)                                                      02340000
C                                                                              02350000
      HUF=0.0                                                                  02360000
      IF(UF.LT.0.0)  HUF=DHIP1-DHOLD                                           02370000
      HUB=DHIM1-DHOLD                                                          02380000
      IF(UB.LT.0.0)  HUB=0.0                                                   02390000
      HWF=0.0                                                                  02400000
      IF(WF.LT.0.0)  HWF=DHJP1-DHOLD                                           02410000
      HWB=DHJM1-DHOLD                                                          02420000
      IF(WB.LT.0.0)  HWB=0.0                                                   02430000
```

```
C                                                                       02440000
C C                                                                     02450000
C                                                                       02460000
      COMP1=DTO2DR*RINV(I)*(HUF*UF-HUB*UB)                              02470000
      COMP2=DTODZ*(HWF*WF-HWB*WB)                                       02480000
      COMP3=FOURMR*RINV(I)*(RHIP1*(TIP1-TOLD)*ADIP1                     02490000
     1-RHIM1*(TOLD-TIM1)*ADIM1)                                         02500000
      COMP4=DTODZ*ALPHA*((TJP1-TOLD)/SURFI*ADJP1-(TOLD-TJM1)/DZ*ADJM1)  02510000
      DEODT=(-COMP1-COMP2+COMP3+COMP4)*RHOINV                           02520000
      DHNEW=DHOLD+DEODT                                                 02540000
      DEDT(I,JMAX)=DEODT/DT                                             02550000
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                         02580000
      ENTH(MN,I,JMAX)=DHNEW                                             02590000
      DEN(MN,I,JMAX)=DD                                                 02600000
      T(MN,I,JMAX)=TNEW                                                 02610000
C                                                                       02620000
C                                                                       02630000
      DO 10 JJ=1,JMAXM2                                                 02640000
      J=JMAX-JJ                                                         02650000
      JP1=J+1                                                           02660000
      JM1=J-1                                                           02670000
      TJP1=TOLD                                                         02680000
      TOLD=TJM1                                                         02690000
      UJP1=UOLD                                                         02700000
      UOLD=UJM1                                                         02710000
      DHJP1=DHOLD                                                       02720000
      DHOLD=DHJM1                                                       02730000
      DJP1=RHO                                                          02740000
      RHO=DJM1                                                          02750000
      TJM1=T(MO,I,JM1)                                                  02760000
      TIP1=T(MO,IP1,J)                                                  02770000
      TIM1=T(MO,IM1,J)                                                  02780000
      UIP1=U(MO,IP1,J)                                                  02790000
      UIM1=U(MO,IM1,J)                                                  02800000
      UJM1=U(MO,I,JM1)                                                  02810000
      PIP1=P(IP1,J)                                                     02820000
```

```
      PIM1=P(IM1,J)                                                    02830000
      PJ=P(I,J)                                                        02840000
      DHJM1=ENTH(MO,I,JM1)                                             02850000
      DHIP1=ENTH(MO,IP1,J)                                             02860000
      DHIM1=ENTH(MO,IM1,J)                                             02870000
      DJM1=DEN(MO,I,JM1)                                               02880000
      DIP1=DEN(MO,IP1,J)                                               02890000
      DIM1=DEN(MO,IM1,J)                                               02900000
      ADIP1=(DIP1+RHO)/2.0D0                                           02910000
      ADIM1=(RHO+DIM1)/2.0D0                                           02920000
      ADJP1=ADJM1                                                      02930000
      ADJM1=(RHO+DJM1)/2.0D0                                           02940000
      RHOINV=1.0D0/RHO                                                 02950000
      UF=RIP1*DIP1*UIP1+RI*RHO*UOLD                                    02960000
      UB=RIM1*DIM1*UIM1+RI*RHO*UOLD                                    02970000
      IF(I.EQ.2) UB=0.0                                                02980000
      IF(I.EQ.IMAX) UF=0.0                                             02990000
      WF=WB                                                            03000000
      WB=DJM1*WW(I,J)                                                  03010000
C     DPDTI=DDDZDT(I,J)*DTODZ                                          03020000
      CALL RMCMEQ                                                      03030000
      U(MN,I,J)=UNEW                                                   03040000
      CALL ENERGY                                                      03050000
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                        03060000
      ENTH(MN,I,J)=DHNEW                                               03070000
      DEN(MN,I,J)=DD                                                   03080000
      T(MN,I,J)=TNEW                                                   03090000
   10 CONTINUE                                                         03100000
      J=1                                                              03110000
      TJP1=TCID                                                        03120000
      TOLD=TJM1                                                        03130000
      UJP1=UOLD                                                        03140000
      UOLD=UJM1                                                        03150000
      DHJP1=DHOLD                                                      03160000
      DHOLD=DHJM1                                                      03170000
      DJP1=RHO                                                         03180000
```

```
      RHO=DJM1                                                          03190000
      TJM1=TBNDS(I)                                                     03200000
      TIP1=T(MO,IP1,1)                                                  03210000
      TIM1=T(MO,IM1,1)                                                  03220000
      UIP1=U(MO,IP1,1)                                                  03230000
      UIM1=U(MO,IM1,1)                                                  03240000
      UJM1=-UOLD                                                        03250000
      PIP1=P(IP1,1)                                                     03260000
      PIM1=P(IM1,1)                                                     03270000
      PJ=P(I,1)                                                         03280000
      DHJM1=HBNDS(I)                                                    03290000
      DHIP1=ENTH(MO,IP1,1)                                              03300000
      DHIM1=ENTH(MO,IM1,1)                                              03310000
      DJM1=DENDS(I)                                                     03320000
      DIP1=DEN(MO,IP1,1)                                                03330000
      DIM1=DEN(MO,IM1,1)                                                03340000
      ADIP1=(DIP1+RHO)/2.0D0                                            03350000
      ADIM1=(RHO+DIM1)/2.0D0                                            03360000
      ADJP1=ADJM1                                                       03370000
      ADJM1=(RHO*DZ+DJM1*CDZ)/(DZ+CDZ)                                  03380000
      RHOINV=1.0D0/RHO                                                  03390000
      UF=RIP1*DIP1*UIP1+RI*RHO*UOLD                                     03400000
      UB=RIM1*DIM1*UIM1+RI*RHO*UOLD                                     03410000
      IF(I.EQ.2) UB=0.0                                                 03420000
      IF(I.EQ.IMAX) UF=0.0                                              03430000
      WF=WB                                                             03440000
      WB=DJM1*WW(I,1)                                                   03450000
C     DPDTI=DDDZDT(I,1)*DTCDZ                                           03460000
      CALL BMCMEQ                                                       03470000
      U(MN,I,1)=UNEW                                                    03480000
```

```
      CALL ENERGY                                                       03490000
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,PJ,XVLIM)                         03500000
      ENTH(MN,I,1)=DHNEW                                                03510000
      DEN(MN,I,1)=DD                                                    03520000
      T(MN,I,1)=TNEW                                                    03530000
11    CONTINUE                                                          03540000
      RETURN                                                            03550000
      END                                                               03560000
```

```
      SUBROUTINE LOOP                                                   03560003
C----                                                                   03560004
C---- LOOP THRU DOWNTAKE AND CALANDRIA.                                 03560005
C---- CALCULATIONS FOR BOTTOM                                           03560006
C----                                                                   03560007
      IMPLICIT REAL*8(A-H,O-Z)                                          03560008
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                 03560009
      REAL*8 IMP(2)                                                     03560010
      COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                03560011
     1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8              03560012
     1,              ENTHFR, FFLUXU                                     03560013
      COMMON/FLAG/ IWSTRT, IFLAG1, IFLAG2                               03560014
      COMMON/ENTLIM/ NVLIM                                              03560015
      COMMON/FORCE/ PUMPDP                                              03560016
      COMMON/MOVE   / DPDT(30)                                          03560017
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       03560018
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 03560019
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   03560020
     3,             SSMAX, SSMIN                                       03560021
      COMMON/PAN/ VOLSCH, RADSQ, VCIC, WVOL, WHEIG                      03560022
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                03560023
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          03560024
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      03560025
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   03560026
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  03560027
     3,             DZODTO                                             03560028
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              03560029
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                03560030
     2,              HVINV,DELHLV,DENSTY                                03560031
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          03560032
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   03560033
     1,             NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             03560034
      COMMON/STEP/MN,MO,N                                               03560035
      COMMON/SIZE/H,RAD,HMAX                                            03560036
      COMMON /AREAP/DV(30),DVOA(30)                                     03560037
```

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      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                03560038
     1,IDWNP1,IDOWM1                                                      03560039
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH     03560040
     1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1              03560041
     2,NCALP1                                                             03560042
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT         03560043
     1,DDDZDT(30,30),DDCDT(10)                                            03560044
      COMMON/VAPDEN/PRESRF,RHOVR                                          03560045
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                03560046
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                               03560047
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)          03560048
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                            03560049
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)          03560050
     1,CALP(10,2)                                                         03560051
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)           03560052
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/           03560053
      EQUIVALENCE (ZZZZ,WDWNJP)                                           03560054
      EQUIVALENCE (ZZZC,CALW)                                             03560055
C                                                                         03560056
CC          RADIAL MOM. EQUATION  LUMPED                                  03560057
C                                                                         03560058
      RHO=DBOTT(MO)                                                       03560059
      RHOINV=1.0D0/RHO                                                    03560060
      UONE=UONEB(MO)                                                      03560061
      UOLD=UBOTT(MO)                                                      03560062
      COMP1=RHOINV*(PBIM1-PBIP1+PUMPDP)*CONST7                            03560063
      COMP2=1.0D0/DT+CONST8*UOLD                                          03560064
      UNEW   = UOLD + COMP1/COMP2*DT                                      03560065
      UBOTT(MM)=UNEW                                                      03560066
C                                                                         03560067
CC          LUMPED ENERGY EQUATIONS                                       03560068
C                                                                         03560069
      DHJP1=HDWNJP(MO)                                                    03560070
      DHOLD=HBOTT(MO)                                                     03560071
      WJM1=WCALJM(MO)                                                     03560072
      DOLD=DBOTT(MO)                                                      03560073
```

```
      BTEODT=ENTHFR/DOLD*(HF*BETA-DHOLD)+DTAUOV*WJM1*(DHJP1-DHOLD)/DT   03560074
      DHNEW=DHOLD+BTEODT*DT                                             03560075
      BTDEDT=BTEODT                                                     03560076
C------  PJ = 50.0 TO PREVENT BOILING (CAUTION)----                    03560077
      CALL CALDEN(DNEW,DHNEW,TNEW,XV,XL,50.0D0,XVLIM)                   03560078
      TCALJM(MN)=TNEW                                                   03560079
      DCALJM(MN)=DNEW                                                   03560080
      HCALJM(MN)=DHNEW                                                  03560081
      CALH(1,MN)=DHNEW                                                  03560082
      CALD(1,MN)=DNEW                                                   03560083
      CALT(1,MN)=TNEW                                                   03560084
      TBOTI(MN)=TNEW                                                    03560085
      DBOTT(MN)=DNEW                                                    03560086
      HBOTT(MN)=DHNEW                                                   03560087
C                                                                       03560088
CC          CALANDRIA                                                   03560089
C                                                                       03560090
      CALL CALHTD                                                       03560091
C                                                                       03560092
CC        SOLVE DIVERGENCE FOR VERTICLE VELOCITIES                      03560093
C                                                                       03560094
      DNEW=DBOTT(MN)                                                    03560095
      UNEW=UBOTT(MN)                                                    03560096
      UONE=CONST6*UNEW                                                  03560097
      UONEB(MN)=UONE                                                    03560098
      WJD=-UONE*ABOAFD                                                  03560099
      WJU=UONE*ABOAFU                                                   03560100
C                                                                       03560101
CC      ADD FEED IN AT BOTTOM NEGLECT MOMMENTUM                         03560102
C                                                                       03560103
      IF(WJU.GT.0.0) GO TO 3232                                         03560104
      IFLAG1=IFLAG1+1                                                   03560105
      IF(IFLAG1.GT.100) STOP 52                                         03560106
      WJU=0.0                                                           03560107
      WJD=0.0                                                           03560108
      WRITE(6,1022) IFLAG1,N                                            03560109
```

```
 1022 FORMAT(1X,'FLOW TENDING IN WRONG DIRECTION  OCCURANCE = '          03560110
     1,I3,'VEL. SET TO ZERO EXEC. CONTINUING',' N=',I6)                 03560111
 3232 CONTINUE                                                          03560112
      WJU=WJU*DNEW                                                      03560113
      WJU=WJU+FFLUXU                                                    03560114
      WDWNJM(MN)=WJD                                                    03560115
      WDWNJP(MN)=WJD                                                    03560116
      WCALJM(MN)=WJU/DNEW                                               03560117
C                                                                       03560118
C                                                                       03560119
C         CALANDRIA                                                     03560120
C         CALCULATE VELOCITY IN TUBES                                   03560121
C                                                                       03560122
C                                                                       03560123
      CALL CALWW                                                        03560124
C                                                                       03560125
      RETURN                                                            03560126
      END                                                               03560127
```

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      SUBROUTINE OUTPUT                                                 03560130
      IMPLICIT REAL*8(A-H,O-Z)                                          03560131
      REAL*8 IMP(2)                                                     03560132
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5), RATH(30)                       03560133
      COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                03560134
     1,             VOLBT, DTADOV, CONST6, CONST7, CONST8              03560135
     1,             ENTHFR, FFLUXU                                     03560136
      COMMON/SIZE/ H,RAD,HMAX                                           03560137
      COMMON /AREAP/ DV(30),DVOA(30)                                    03560138
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               03560139
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         03560140
      COMMON/INOUT/IN,IOUT                                              03560141
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)              03560142
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                             03560143
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)        03560144
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                          03560145
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)       03560146
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                 03560147
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                   03560148
     3,             SSMAX, SSMIN                                       03560149
      COMMON/GRID/ DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ     03560150
     1,            DT2DRZ,DTODRZ,DTCDR,FOURMD,DZORSQ,DZODT,DTORSQ      03560151
     2,            DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO     03560152
     3,            DZODTO                                              03560153
      COMMON/REAL/ RTIME,TCONST                                         03560154
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      03560155
      COMMON/DIMEN/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           03560156
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                03560157
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          03560158
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              03560159
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                03560160
     2,             HVINV,DELHLV,DENSTY                                03560161
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          03560162
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   03560163
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             03560164
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      COMMON/STEP/MN,MO,N                                                    03560165
      COMMON/AVPART/AVERNN(2),AVERLL(2)                                      03560166
      COMMON/CHEST/UU,UA,TUBEH,AREAT,FOA,UFOA,DTOTH,THODT,UAOA,CALANH        03560167
     1,BOTTH,TUBED,FMGM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                 03560168
     2,NCALP1                                                                03560169
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                        03560170
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                    03560171
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)             03560172
     1,CALP(10,2)                                                            03560173
      EQUIVALENCE (ZZZZ,WDWNJP)                                              03560174
      EQUIVALENCE (ZZZC,CALW)                                                03560175
      WRITE(6,1000)  N,RTIME                                                 03560176
      WRITE(6,1020)                                                          03560177
      WRITE(6,1013)                                                          03560178
      DO 1 JJ=1,JMAXP1                                                       03560179
      J=JMAXP2-JJ                                                            03560180
    1 WRITE(6,1001) (U(MN,I,J),I=2,IMAX)                                     03560181
      WRITE(6,1014)                                                          03560182
      WRITE(6,1001) (W(MN,I,JMAXP2),I=2,IMAX)                                03560183
      DO 2 JJ=1,JMAXP1                                                       03560184
      J=JMAXP2-JJ                                                            03560185
    2 WRITE(6,1001) (W(MN,I,J),I=2,IMAX)                                     03560186
      WRITE(6,1015)                                                          03560187
      WRITE(6,1001) (FRAT(I),I=2,IMAX)                                       03560188
      DO 22 JJ=1,JMAXP1                                                      03560189
      J=JMAXP2-JJ                                                            03560190
   22 WRITE(6,1001) (WW(I,J),I=2,IMAX)                                       03560191
      WRITE(6,1016)                                                          03560192
      DO 3 JJ=1,JMAXP2                                                       03560193
      J=JMAXP2-JJ+1                                                          03560194
    3 WRITE(6,1001) (P(I,J),I=2,IMAX)                                        03560195
      WRITE(6,1017)                                                          03560196
      DO 4 JJ=1,JMAXP2                                                       03560197
      J=JMAXP2-JJ+1                                                          03560198
    4 WRITE(6,1001) (T(MN,I,J),I=2,IMAX)                                     03560199
      WRITE(6,1018)                                                          03560200
```

```
      DO 5 JJ=1,JMAXP2                                                  03560201
      J=JMAXP2-JJ+1                                                     03560202
    5 WRITE(6,1001) (ENTH(MN,I,J),I=2,IMAX)                             03560203
      WRITE(6,1019)                                                     03560204
      DO 6 JJ=1,JMAXP2                                                  03560205
      J=JMAXP2-JJ+1                                                     03560206
    6 WRITE(6,1001) (DEN(MN,I,J),I=2,IMAX)                              03560207
      WRITE(6,1004)                                                     03560208
      WRITE(6,1008)                                                     03560209
      WRITE(6,1005) (ZZZZ(MN,I),I=1,4)                                  03560210
C     WRITE(6,1009)                                                     03560211
C     WRITE(6,1005) ZZZZ(MN,5)                                          03560212
      WRITE(6,1010)                                                     03560213
      WRITE(6,1005)  ZZZZ(MN,9),(ZZZZ(MN,I),I=6,8)                      03560214
C     WRITE(6,1007)  ZZZZ(MN,10)                                        03560215
      WRITE(6,1011)                                                     03560216
      WRITE(6,1005) (ZZZZ(MN,I),I=11,14)                                03560217
      WRITE(6,1012)                                                     03560218
      WRITE(6,1005) (ZZZZ(MN,I),I=15,18)                                03560219
      WRITE(6,1002)                                                     03560220
      WRITE(6,1006) PBIM1,PBIP1                                         03560221
      WRITE(6,1003)                                                     03560222
      WRITE(6,1021)                                                     03560223
      WRITE(6,1014)                                                     03560224
      WRITE(6,1001) (CALW(J,MN),J=1,NCAL)                               03560225
      WRITE(6,1016)                                                     03560226
      WRITE(6,1001) (CALP(J,MN),J=1,NCAL)                               03560227
      WRITE(6,1017)                                                     03560228
      WRITE(6,1001) (CALT(J,MN),J=1,NCAL)                               03560229
      WRITE(6,1018)                                                     03560230
      WRITE(6,1001) (CALH(J,MN),J=1,NCAL)                               03560231
      WRITE(6,1019)                                                     03560232
      WRITE(6,1001) (CALD(J,MN),J=1,NCAL)                               03560233
C                                                                       03560234
      RETURN                                                            03560235
```

```
      ENTRY OUTALL                                                      03560236
      WBAR=0.0                                                          03560237
      UBAR=0.0                                                          03560238
      RATZ  = DDZDT*DFLOAT(JMAX)                                        03560239
      DO 90 I=2,IMAX                                                    03560240
      RATH(I)  =  W(MN,I,JMAXP2) - RATZ                                 03560241
      DO 90 J=1,JMAXP1                                                  03560242
      UBAR=UBAR+DABS(U(MN,I,J)-U(MO,I,J))                               03560243
      WBAR=WBAR+DABS(W(MN,I,J)-W(MO,I,J))                               03560244
   90 CONTINUE                                                          03560245
      FRACH=HH(MN)/HMAX                                                 03560246
      WRITE(6,1003)                                                     03560247
      WRITE(6,1029)                                                     03560248
      WRITE(6,1001) (SURFAC(I),I=2,IMAX)                                03560249
      WRITE(6,1031)                                                     03560250
      WRITE(6,1001) (RATH(I),I=2,IMAX)                                  03560251
      WRITE(6,1003)                                                     03560252
      WRITE(6,1023)  TMASS(MN),XSP(MN),XIP(MN),XCP(MN),XWP(MN)          03560253
      WRITE(6,1024)  AVERT(MN),AVERH(MN),AVERD(MN)                      03560254
      WRITE(6,1025)  AVERNN(MN), AVERLL(MN)                             03560255
      WRITE(6,1030)  G(MN), SSMAX, SSMIN                                03560256
      WRITE(6,1026)  HH(MN), FRACH, EM(MN), Q(MN), EMVINT               03560257
      WRITE(6,1027)  UBAR, WBAR, DZ, DDZDT                              03560258
      WRITE(6,1028)  HHH(MN), HHM(MN), E(MN), EVINTO                    03560259
CFORMATS                                                                03560260
 1000 FORMAT(1H1,'  N= ',I10,2X,'REAL TIME = ',F10.2,' SEC.',/)         03560261
 1001 FORMAT(11(1X,G11.4),/)                                            03560262
 1002 FORMAT(/)                                                         03560263
 1003 FORMAT(//)                                                        03560264
 1004 FORMAT(//,10X,'CONDITIONS IN BOTTOM',/)                           03560265
 1005 FORMAT(6X,'VEL=',G11.4,1X,'TEMP=',G11.4,1X,'DEN=',G11.4           03560266
     1,1X,'ENTHAL=',G11.4,/)                                            03560267
 1006 FORMAT(1X,'PRESSURE AT DWNTAKE=',G11.4,'PRESSURE AT UP'           03560268
     1,'TAKE=',G11.4)                                                   03560269
 1007 FORMAT(6X,'VEL*=',G11.4)                                          03560270
 1008 FORMAT(4X,'TOP OF DOWNTAKE',/)                                    03560271
```

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1009 FORMAT(4X,'BOTTOM OF DOWNTAKE',/)                                  03560272
1010 FORMAT(4X,'BOTTOM OF PAN',/)                                       03560273
1011 FORMAT(4X,'AVERAGE CONDITIONS IN STEAM CHEST',/)                   03560274
1012 FORMAT(4X,'BOTTOM OF STEAM CHEST',/)                               03560275
1013 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF RADIAL VELOCITY',/)           03560276
1014 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF VERTICAL VELOCITY',/)         03560277
1015 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF VERTICAL VELOCITY INTO'       03560278
    1,' EACH MOVING CELL',/)                                            03560279
1016 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF PRESSURE',/)                  03560280
1017 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF TEMPERATURE',/)               03560281
1018 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF ENTHALPY',/)                  03560282
1019 FORMAT(/,8X,'SPATIAL DISTRIBUTION OF DENSITY',/)                   03560283
1020 FORMAT(/,10X,'CONDITIONS ABOVE THE CALANDRIA',/)                   03560284
1021 FORMAT(10X,'CONDITIONS IN TUBES BOTTOM TO TOP',/)                  03560285
1022 FORMAT(10X,'AVERAGE CONDITIONS IN PAN',/)                          03560286
1023 FORMAT(5X,'TOTAL MASS =',G12.5,/                                   03560287
    1,5X,'MASS FRACTIONS:',2X,'SOLUT. SUGAR=',E10.3,2X,'IMPURITY='      03560288
    2,E10.3,2X,'CRYSTAL=',E10.3,2X,'WATER=',E10.3,/)                    03560289
1024 FORMAT(5X,'TEMPERATURE=',E14.7,' ENTHALPY=',E14.7                  03560290
    1,' DENSTIY=',E14.7,/)                                              03560291
1025 FORMAT(5X,'NUMBER OF CRYSTALS=',E14.7,2X,'AVERAGE LENGHT=',E14.7   03560292
    1,' FEET'/)                                                         03560293
1026 FORMAT(5X,'LEVEL=',F5.2,' FT.',' PREC.MAX=',F5.2,' EVAP. RATE='    03560294
    1,G11.4,' HEAT IN=',G11.4,' TOTAL EVAP.=',G11.4,/)                  03560295
1027 FORMAT(10X,'UBAR=',G11.4,' WBAR=',G11.5,' DZ=',G11.4               03560296
    1,' DDZDT=',G11.4,/)                                                03560297
1028 FORMAT(10X,'DOUBLE CHECK FORM OVERALL BALANCES'/                   03560298
    1,6X,'HHH=',G11.4,' HHM=',G11.4,' E=',G11.4                         03560299
    2,6X,'TOTAL E =',G11.4)                                             03560300
1029 FORMAT(10X,'SURFACE HEIGHTS',/)                                    03560301
1030 FORMAT(5X,'AV. GROWTH RATE= ',E9.2,' MAX. SUPERSAT.= ',F4.2        03560302
    1,' MIN. SUPERSAT.= ',F4.2,/)                                       03560303
1031 FORMAT(/,10X,'RATE OF CHANGE OF SURFACE HEIGHTS',/)                03560304
     RETURN                                                             03560305
     END                                                                03560306
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      SUBROUTINE PARMEQ                                                 03560309
C-----                                                                  03560310
C----- PROFORMS NON-DIMENSIONALIZATION OF ANY                           03560311
C----- DIMENSIONAL PARMATERS OR REDEFINES PARMATERS TO                  03560312
C----- CONSISTENT WITH CALCULATIONS.                                    03560313
C-----                                                                  03560314
      IMPLICIT REAL*8 (A-H,O-Z)                                         03560315
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                           03560316
     1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                 03560317
      COMMON / SIZE/   H , RAD, HMAX                                    03560318
      COMMON / PARS/   PARS1, PARS2, PARS3, PARS4, PARS5                03560319
      COMMON / SPARS/ SPARS1, SPARS2, SPARS3, SPARS4, SPARS5            03560320
      COMMON / PARV/ PARV1, PARV2, PARV3, PARV4                         03560321
      COMMON / SPARV/ SPARV1, SPARV2, SPARV3, SPARV4                    03560322
      COMMON / PARH/  PARH1, PARH2, PARH3, PARH4,                       03560323
     &                PARH5, PARH6, PARH7, PARH8                       03560324
      COMMON / SPARH/ SPARH1, SPARH2, SPARH3, SPARH4,                   03560325
     &                SPARH5, SPARH6, SPARH7, SPARH8, SPARH9           03560326
      COMMON / PARG/ PARG1, PARG2, PARG3, PARG4,                        03560327
     &               PARG5, PARG6, PARG7, PARG8, PARG9                  03560328
      COMMON / SPARG/ SPARG1, SPARG2, SPARG3, SPARG4,                   03560329
     &                SPARG5, SPARG6                                   03560330
      COMMON / PART/ PART1, PART2, PART3                                03560331
      COMMON / SPART/ SPART1, SPART2, SPART3                            03560332
      COMMON / PRATIO/ PARR1, PARR2, PARR3                              03560333
      COMMON / PARCP/ PRCP1, PRCP2, PRCP3, PRCP4                        03560334
      COMMON / PARBP/ PRBP1, PRBP2                                      03560335
      COMMON / SPRATO/ SPARR1, SPARR2, SPARR3                           03560336
      COMMON / SPARCP/ SPRCP1, SPRCP2, SPRCP3, SPRCP4                   03560337
      COMMON / SPARBP/ SPRBP1, SPRBP2                                   03560338
      COMMON / VAPDEN / PRESRF, RHOVR                                   03560339
      COMMON / UNITS/ DIMVIS, DIMPRS                                    03560340
      COMMON/PROPTY/ RHO,RHOINV,RHOC2,VISC,ALPHA,VORHO,BETA             03560341
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                03560342
     2,             HVINV,DELHLV,DENSTY                                03560343
      NAMELIST /SUPST/ PARS1, PARS2, PARS3, PARS4, PARS5                03560344
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      NAMELIST /SUPSTS/ SPARS1, SPARS2, SPARS3, SPARS3, SPARS5          03560345
      NAMELIST /GROW / PARG1, PARG2, PARG3, PARG4, PARG5,               03560346
     &                 PARG6, PARG7, PARG8, PARG9                       03560347
      NAMELIST /GROWS / SPARG1, SPARG2, SPARG3, SPARG3, SPARG5,         03560348
     &                  SPARG6                                          03560349
      NAMELIST /VAPOR/ PARH1, PARH2, PARH3, PARH4, PARH5,               03560350
     &                 PARH6, PARH7, PARH8, PARH9                       03560351
      NAMELIST /VAPORS/ SPARH1, SPARH2, SPARH3, SPARH3, SPARH5,         03560352
     &                  SPARH6, SPARH7, SPARH8, SPARH9                  03560353
      NAMELIST /VISTY/ PARV1, PARV2, PARV3, PARV4                       03560354
      NAMELIST /VISTYS/ SPARV1, SPARV2, SPARV3, SPARV4                  03560355
      NAMELIST /SATTM/ PART1, PART2, PART3                              03560356
      NAMELIST /SATTMS/ SPART1, SPART2, SPART3                          03560357
      NAMELIST /CONSTS/ DIMPRS, DIMVIS, PRESRF, HMAX                    03560358
      NAMELIST  /VRATO/   PARR1, PARR2, PARR3                           03560359
      NAMELIST  / SUGCP/  PRCP1, PRCP2, PRCP3, PRCP4                    03560360
      NAMELIST  / SUGBPE/ PRBP1, PRBP2                                  03560361
      NAMELIST  /SVRATO/  SPARR1, SPARR2, SPARR3                        03560362
      NAMELIST  /SSUGCP/  SPRCP1, SPRCP2, SPRCP3, SPRCP4                03560363
      NAMELIST  /SSUGBP/  SPRBP1, SPRBP2                                03560364
C                                                                       03560365
      WRITE(6,CONSTS)                                                   03560366
C                                                                       03560367
C                                                                       03560368
      SPARS1   = PARS1 + (PARS2+TZERO*PARS3+TZERO*TZERO*PARS4)*TZERO    03560369
      SPARS2   = (PARS2 + 2.0D0*TZERO*PARS3+3.0D0*TZERO**2*PARS4)/BETA  03560370
      SPARS3   = (PARS3 + 3.0D0*TZERO*PARS4)/BETA/BETA                  03560371
      SPARS4   = PARS4/BETA/BETA/BETA                                   03560372
      SPARS5   = PARS5                                                  03560373
C                                                                       03560374
      DDLOG    = DLOG(DIMVIS)                                           03560375
      SPARV1   = PARV1*BETA                                             03560376
      SPARV2   = (PARV2 + TZERO)*BETA                                   03560377
      SPARV3   = PARV3                                                  03560378
      SPARV4   = PARV4 - DDLOG                                          03560379
```

```
C                                                                       03560380
      DELTZ    = TZERO-32.0D0                                           03560381
      SPARH1   = (PARH1 - HR +                                          03560382
     &  (PARH2 + PARH3*DELTZ + PARH4*DELTZ**2)*DELTZ)*BETA              03560383
      SPARH2   = PARH2 + ( 2.0D0*PARH3 + 3.0D0*DELTZ*PARH4)*DELTZ       03560384
      SPARH3   = (PARH3 + 3.0D0*DELTZ*PARH4)/BETA                       03560385
      SPARH4   = PARH4/BETA/BETA                                        03560386
      SPARH5   = DIMPRS*(PARH5 + 2.0D0*DIMPRS*PRESRF*PARH7)             03560387
      SPARH6   = PARH6 +                                                03560388
     &  (PARH5 + PARH7*DIMPRS*PRESRF)*DIMPRS*PRESRF                     03560389
      SPARH7   = PARH7*DIMPRS*DIMPRS                                    03560390
      SPARH8   = PARH8*DIMPRS/BETA                                      03560391
      SPARH9   = PARH8/BETA*DIMPRS*PRESRF                               03560392
C                                                                       03560393
      SPARG1   = (PARG1 + TZERO*PARG2 + PARG3*PARG2)/PARG5*BETA*PARG6   03560394
      SPARG2   = PARG2 /PARG5 * PARG6                                   03560395
      SPARG3   = PARG4 /PARG5 * BETA*PARG6                              03560396
      SPARG4   = (PARG7 + TZERO)*BETA                                   03560397
      SPARG5   = 1.0D0/PARG8/BETA/PARG6                                 03560398
      SPARG6   = PARG9                                                  03560399
C                                                                       03560400
      SPART1   = PART1*BETA                                             03560401
      SPART2   = PART2 - DLOG10(DIMPRS)                                 03560402
      SPART3   = (PART3 - TZERO)*BETA                                   03560403
C                                                                       03560404
      SPRCP1   = PRCP1                                                  03560405
      SPRCP2   = PRCP2*PRCP3                                            03560406
      SPRCP3   = PRCP2/PRCP4                                            03560407
C                                                                       03560408
      SPARR1   = PARR1                                                  03560409
      SPARR2   = PARR2                                                  03560410
      SPARR3   = PARR3                                                  03560411
C                                                                       03560412
      SPRBP1   = PRBP1                                                  03560413
      SPRBP2   = PRBP2                                                  03560414
      WRITE(6,SUPST)                                                    03560415
```

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      WRITE(6,SUPSTS)                                                   03560416
      WRITE(6,GROW )                                                    03560417
      WRITE(6,GROWS )                                                   03560418
      WRITE(6,VAPOR)                                                    03560419
      WRITE(6,VAPORS)                                                   03560420
      WRITE(6,VISTY)                                                    03560421
      WRITE(6,VISTYS)                                                   03560422
      WRITE(6,SATTM)                                                    03560423
      WRITE(6,SATTMS)                                                   03560424
      WRITE(6,SUGBPE)                                                   03560425
      WRITE(6,SSUGBP)                                                   03560426
      WRITE(6,SUGCP)                                                    03560427
      WRITE(6,SSUGCP)                                                   03560428
      WRITE(6,VRATO)                                                    03560429
      WRITE(6,SVRATO)                                                   03560430
      RETURN                                                            03560431
      END                                                               03560432
```

```
      SUBROUTINE PRELIM                                                 03560435
C----                                                                   03560436
C----  PREFORMS ANY INITIALIZATION CR PRELIMINARY CALCULATIONS.         03560437
C----  READS IN DATA FOR RUN.                                           03560438
C----                                                                   03560439
      IMPLICIT REAL*8(A-H,O-Z)                                          03560440
      INTEGER STMODE                                                    03560441
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5),QFLUX(10)                       03560442
      DIMENSION ZPARS(5),ZPARV(4),ZPARH(8),ZPARG(9),ZPART(3)            03560443
      DIMENSION ZPARCP(4),ZPARBP(2),ZRATIO(3)                           03560444
      REAL*8 IMP(2)                                                     03560445
      COMMON/JOBRUN/ IRUN(3)                                            03560446
      COMMON/UNITS   / DIMVIS, DIMPRS                                   03560447
      COMMON/ CHECK/ DELHIO(30),DELHT(30),DELHDT(30),DELWIO(30)         03560448
      COMMON/BOTTOM/ VOLUP, AFLWU, AFLWD, ABOAFD, ABOAFU                03560449
     1,              VOLBT, DTAUOV, CONST6, CONST7, CONST8              03560450
     1,              ENTHFR, FFLUXU                                     03560451
      COMMON/MOVE   / DPDT(30)                                          03560452
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               03560453
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)              03560454
     1,WDWNJM(2),TBOTT(2),DBOTT(2),HBOTT(2)                             03560455
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)        03560456
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                          03560457
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)        03560458
     1,CALP(10,2)                                                       03560459
      COMMON/REAL/ RTIME, TCONST                                        03560460
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           03560461
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                03560462
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                          03560463
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          03560464
      COMMON/STEP/MN,MC,N                                               03560465
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT       03560466
     1,DDDZDT(30,30),DDCDT(10)                                          03560467
      COMMON /AREAP/DV(30),DVOA(30)                                     03560468
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO         03560469
      COMMON/FORCE/ PUMPDP                                              03560470
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      COMMON/INOUT/IN,IOUT                                                    03560471
      COMMON/ESTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),BEM(2),HH(2)             03560472
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                       03560473
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                         03560474
     3,          SSMAX, SSMIN                                                 03560475
      COMMON/FLAG/ IWSTRT, IFLAG1, IFLAG2                                     03560476
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                            03560477
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ            03560478
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                         03560479
     2,DZO2,CALFC2,CALFC3,DDZDT,SUBFDT,DET2,DZO,DDZDTO                        03560480
     3,          DZODTO                                                       03560481
      COMMON/PROPTY/RHO,RHOINV,RHOC2,VISC,ALPHA,VORHO,BETA                    03560482
     1,           FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                        03560483
     2,           HVINV,DELHLV,DENSTY                                        03560484
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT         03560485
     1,           NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1                     03560486
      COMMON/SIZE/H,RAD,HMAX                                                  03560487
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH         03560488
     1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAI,NCALM1                  03560489
     2,NCALP1                                                                 03560490
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                    03560491
     1,IDWNP1,IDOWM1                                                          03560492
      COMMON/AVPART/AVERNN(2),AVERLL(2)                                       03560493
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                         03560494
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                     03560495
      COMMON/ENTLIM/XVLIM                                                     03560496
      COMMON/VAPDEN/PRESRF,RHOVR                                              03560497
      COMMON/ EMPEQ/ SLIPV, FXPV                                              03560498
      COMMON/ ITTER/ NSITER                                                   03560499
      COMMON/ EQUTON / RATCR                                                  03560500
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                                 03560501
     1      VART, PRECMX, AHTOV, HR, TINTAL, HV, JJMAX                        03560502
      COMMON / PARS/    PARS1, PARS2, PARS3, PARS4, PARS5                     03560503
      COMMON / PARV/ PARV1, PARV2, PARV3, PARV4                               03560504
      COMMON / PARH/  PARH1, PARH2, PARH3, PARH4,                             03560505
     &                PARH5, PARH6, PARH7, PARH8                             03560506
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      COMMON / PARG/ PARG1, PARG2, PARG3, PARG4,                        03560507
     &               PARG5, PARG6, PARG7, PARG8, PARG9                  03560508
      COMMON / PART/ PART1, PART2, PART3                                03560509
      COMMON / PRATIO/ PARR1, PARR2, PARR3                              03560510
      COMMON / PARCP/ PRCP1, PRCP2, PRCP3, PRCP4                        03560511
      COMMON / PARBP/ PRBP1, PRBP2                                      03560512
      DATA GR,PIE,RHOC/32.2D0,3.14159D0,99.1D0/                         03560513
      EQUIVALENCE (ZZZZ,WDWNJP)                                         03560514
      EQUIVALENCE (ZZZC,CALW)                                           03560515
      EQUIVALENCE (ZPARS,PARS1)                                         03560516
      EQUIVALENCE (ZPARV,PARV1)                                         03560517
      EQUIVALENCE (ZPARH,PARH1)                                         03560518
      EQUIVALENCE (ZPARG,PARG1)                                         03560519
      EQUIVALENCE (ZPART,PART1)                                         03560520
      EQUIVALENCE (ZPARCP,PRCP1)                                        03560521
      EQUIVALENCE (ZPARBP,PRBP1)                                        03560522
      EQUIVALENCE (ZRATIO,PARR1)                                        03560523
C------- DEFINE THE PAN                                                 03560524
      NAMELIST /DDPAN/ RAD, PRECMX, WVOL, WHEIG,                        03560525
     1     AHTOV, TUBEH, TUBED,                                         03560526
     2     IMAX, JJMAX, IDOWN,                                          03560527
     3     ILEFT, IRIGHT, NCAL                                          03560528
C------   REFERENCE PHYISICAL PROPERTIES                               03560529
      NAMELIST /PHYSP/ BETA, DELDDB, BRIXR,                             03560530
     1     RHOVR, DENSTY, TZERO,                                        03560531
     2     HV, DELHLV, HR                                               03560532
C------   LOAD VARIABLES - THINGS THAT CHANGE                          03560533
      NAMELIST /LOADV/ F, BRIXFF, PURFF,                                03560534
     1     TEMPFF, TSTEAM, UU, PRESRF, EVAP                             03560535
C------   INITIALIZATION VARIABLES                                     03560536
      NAMELIST /INTIAL/ XSP, XIP, XCP, XWP,                             03560537
     1     AVERLL, AVERNN,                                              03560538
     2     RATCR, TINTAL                                                03560539
C------   VARIABLES NEEDED FOR COMPUTATIONAL PURPOSES                  03560540
      NAMELIST /STABLE/ MSITER, SFSMTH, THETAZ, THETAS,                 03560541
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     1     XVLIM, SLIPV, EXPV,                                              03560542
     2     PUMPDP, VART, ALPHA,                                             03560543
     3     IWSTRT, DT                                                       03560544
C--------- PARAMETERS FOR FUNCTIONS                                        03560545
      NAMELIST /SUPST/ PARS1, PARS2, PARS3, PARS4, PARS5                   03560546
      NAMELIST /GROW / PARG1, PARG2, PARG3, PARG4, PARG5,                  03560547
     &                 PARG6, PARG7, PARG8, PARG9                        03560548
      NAMELIST /VAPOR/ PARH1, PARH2, PARH3, PARH4, PARH5,                  03560549
     &                 PARH6, PARH7, PARH8, PARH9                        03560550
      NAMELIST /VISTY/ PARV1, PARV2, PARV3, PARV4                          03560551
      NAMELIST /SATTM/ PART1, PART2. PART3                                 03560552
      NAMELIST  /VRATO/   PARR1, PARR2, PARR3                              03560553
      NAMELIST  / SUGCP/  PRCP1, PRCP2, PRCP3, PRCP4                       03560554
      NAMELIST  / SUGBPE/ PRBP1, PRBP2                                     03560555
C                                                                          03560556
C------  RUN IDENTIFICATION                                                03560557
      READ(5,1006) IRUN                                                    03560558
 1006 FORMAT(3A4)                                                          03560559
C------  IN- INPUT UNIT NO.  IOUT- OUTPUT UNIT NO.                         03560560
      READ(5,*) IN,IOUT                                                    03560561
      WRITE(6,1002) IN,IOUT                                                03560562
C------   STMODE- STARTING MODE                                            03560563
C------  .EQ. 1   COLD START                                               03560564
C------  .NE. 1   RESTART                                                  03560565
      READ(5,*) STMODE                                                     03560566
      WRITE(6,1002) STMODE                                                 03560567
C------  NMAX - MAX. NO. OF TIME STEPS                                     03560568
C------  NPRINT- PRINT INTERVAL FOR BIG PRINTOUT                           03560569
C------  NEAR  - PRINT INTERVAL FOR SMALL PRINTOUT                         03560570
C------  NSTART - TIME STEP WHEN PRINTOUTS START                           03560571
      READ(5,*) NMAX,NPRINT,NEAR,NSTART                                    03560572
      WRITE(6,1002) NMAX,NPRINT,NEAR,NSTART                                03560573
      IF(STMODE.EQ.1) GO TO 600                                            03560574
      REWIND IN                                                            03560575
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      READ(IN,1111) U,W,T,P,ENTH,DEN,DUDT,DEDT,ZZZZ,WW,HCDT          03560576
     1,ZZZC,DHDT,SURFAC,H,RAD,HMAX,BTDUDT,BTDEDT                     03560577
     1,DDDZDT,DDCDT                                                  03560578
     2,EM,S,IMP,C,Q,AVERT,HH,F,BRIXFF,PURFF,TEMPFF                   03560579
     3,G,TMASS,WATER,AVERD                                           03560580
     4,AVERH,RTIME,VOLSCH,RADSQ,VOLC,WVOL,WHEIG,AREAT                03560581
     5,DT,DR,DZ,CDZ,DDZDT,SURFDT                                     03560582
     6,BETA,AVERNN,AVERLL                                            03560583
     7,DENSTY,SLIPV,EXPV,VART,HR,ALPHA,SFSMTH                        03560584
     X,UU,UA,TUBEH,POA,UPOA,TUBED,CALANH,TSTEAM,TZERO                03560585
     X,FRAT,BOTTH,RATCR                                              03560586
     X,RHOVR,PRESRF,DELDDB,BRIXR                                     03560587
     X,TOTALH,XSP,XIP,XCP,XWP,PBIP1,PBIM1                            03560588
     1,ZPARS,   ZPARV,   ZPARH,   ZPARG,   ZPART                     03560589
     2,ZPARCP,   ZPAREP,   ZRATIO                                    03560590
      READ(IN,1113) IMAX,JMAX,IRIGHT,ILEFT,IDOWN,MN,MC               03560591
     9,NTUBES,NCAL                                                   03560592
 1111 FORMAT(250A8,250A8,250A8,250A8,250A8,250A8,250A8,250A8,250A8   03560593
     1,133A8)                                                        03560594
 1113 FORMAT(19A4)                                                   03560595
C                                                                    03560596
C-------------------------------------------------------------------- 03560597
C--------    U         - RADIAL VELOCITY                             03560598
C--------    W         - VERTICAL VELOCITY                           03560599
C--------    T         - TEMPERATURE                                 03560600
C--------    P         - PRESSURE                                    03560601
C--------    ENTH      - ENTHALPY                                    03560602
C--------    DEN       - DENSTITY                                    03560603
C--------    DUDT      - TIME DERIVATIVE OF U                        03560604
C--------    DEDT      - TIME DERIVATIVE OF ENTH                     03560605
C--------    HCDT      - TIME DERIVATIVE OF ENTH CALANDRIA           03560606
C--------    DHDT      - TIME DERIVATIVE OF SURFACE HEIGHT           03560607
C--------    H,(HH)    - AVERAGE SURFACE HEIGHT                      03560608
C--------    RAD       - PAN RADIUS                                  03560609
C--------    HMAX      - MAX. PAN HEIGHT                             03560610
C--------    SURFAC    - SURFACE CELL HEIGHT                         03560611
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C--------  E,(EM)    - EVAPORATION RATE                                    03560612
C--------  S         - TOTAL MASS OF DISOLVED SUGAR                        03560613
C--------  IMP       - TOTAL MASS OF IMPURITY                              03560614
C--------  C         - TOTAL MASS OF CRYSTALS                              03560615
C--------  Q         - HEAT INPUT RATE                                     03560616
C--------  AVERT     - AVERAGE TEMPERATURE IN PAN                          03560617
C--------  F         - FEED RATE                                           03560618
C--------  BRIXXF    - BRIX OF FEED                                        03560619
C--------  PURFF     - PURITY OF FEED                                      03560620
C--------  TEMPFF    - TEMPERATURE OF FEED                                 03560621
C--------  G         - GROWTH RATE                                         03560622
C--------  TMASS     - TOTAL MASS IN PAN                                   03560623
C--------  WATER     - TOTAL MASS OF WATER                                 03560624
C--------  AVERD     - AVERAGE DENSITY IN PAN                              03560625
C--------  AVERH     - AVERAGE ENTHALPY IN PAN                             03560626
C--------  RTIME     - REAL TIME                                           03560627
C--------  VOLSCH    - VOLUME OF THE STEAM CHEST(CALANDRIA)                03560628
C--------  RADSQ     - RADIUS SQUARED                                      03560629
C--------  VOLC      - VOLUME OF PAN BELOW PAN PROPER                      03560630
C--------  WVOL      - WORKING VOLUME OF PAN                               03560631
C--------  WHEIG     - WORKING HEIGHT OF PAN                               03560632
C--------  PRECMX    - PRECENT OF MAX. HEIGHT OF PAN                       03560633
C--------  AREAT     - HEAT TRANSFER AREA                                  03560634
C--------  AHTOV     - RATIO OF THE HEAT TRANSFER AREA TO VOLUME           03560635
C--------  DT        - TIME STEP                                           03560636
C--------  DR        - RADIAL INCREMENT                                    03560637
C--------  DZ        - VERTICAL INCREMENT                                  03560638
C--------  CDZ       - VERTIACL INCREMENT IN THE CALANDRIA                 03560639
C--------  DDZDT,(SURFDT) - RATE OF CHANGE VERTICAL INCREMENT              03560640
C--------  BETA      - COEFFICIENT OF THERMAL EXPANSION                    03560641
C--------  AVERNN    - AVERAGE NO. DENSITY OF CRYSTALS                     03560642
C--------  AVERLL    - AVERAGE CRYSTAL SIZE                                03560643
C--------  DENSTY    - REFERENCE DENSITY                                   03560644
C--------  SLIPV     - PARMETER FOR SLIP VELOCITY OF VAPOR AT SURFACE      03560645
C--------  EXPV      - PARMETER FOR SLIP VELOCITY OF VAPOR AT SURFACE      03560646
C--------  VART      - ARTIFICIAL VISCOSITY(=0)                            03560647
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C--------   HR       - REFERENCE ENTHALPY OF LIQUID                          03560648
C--------   ALPHA    - THERMAL DIFFUSIVITY                                   03560649
C--------   SFSMTH   - SURFACE DIFFUSIVITY (SMOOTH FACTER)                   03560650
C--------   UU       - HEAT TRANSFER COEFFICIENT                             03560651
C--------   TSTEAM   - STEAM TEMPERATURE                                     03560652
C--------   TZERO    - INITIAL TEMPERATURE IN PAN                            03560653
C--------   RATCR    - GROWTH RATE CONSTANT                                  03560654
C--------   RHOVR    - REFERENCE DENSITY OF VAPOR                            03560655
C--------   PRESRF   - PRESSURE IN VAPOR SPACE                               03560656
C--------   DELDDB   - COEFFICIENT OF CONCENTRATION                          03560657
C--------   BRIXR    - REFERENCE BRIX                                        03560658
C--------   XSP      - MASS FRACTION SUGAR                                   03560659
C--------   XIP      - MASS FRACTION IMPURITY                                03560660
C--------   XCP      - MASS FRACTION CRYSTAL                                 03560661
C--------   XWP      - MASS FRACTION WATER                                   03560662
C--------   IWSTRT   - EQ. 1   DO WSTRT CALCULATIONS                         03560663
C--------            - GT. 1   DO NOT DO  WSTRT CALCULATIONS                 03560664
C--------   IMAX     - NO. RADIAL GRID POINTS                                03560665
C--------   JMAX     - NO. OF SUBSURFACE CELLS                               03560666
C--------   IRIGHT   - RIGHT MOST RADIAL GRID POINT CONTAINING CALANDRIA     03560667
C--------   ILEFT    - LEFT MOST RADIAL GRID POINT CONTAINING CALANDRIA      03560668
C--------   IDOWN    - RIGHT MOST RADIAL GRID POINT IN DOWNTAKE              03560669
C--------   NCAL     - NO. OF GRID POINTS IN CALANDRIA                       03560670
C--------   TUBEH    - HEIGHT OF TUBES                                       03560671
C--------   TUBED    - DIAMETER OF TUBES                                     03560672
C--------   NTUBES   - NO. OF TUBES                                          03560673
C--------   BOTTH    - HEIGHT OF THE BOTTOM OF PAN TO CALANDRIA              03560674
 600  CONTINUE                                                               03560675
C                                                                           03560676
      READ(5,DDPAN)                                                         03560677
      READ(5,PHYSP)                                                         03560678
      READ(5,LOADV)                                                         03560679
      READ(5,INTIAL)                                                        03560680
      READ(5,STABLE)                                                        03560681
      READ(5,SUPST)                                                         03560682
      READ(5,GROW)                                                          03560683
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      READ(5,VAPOR)                                                    03560684
      READ(5,VISTY)                                                    03560685
      READ(5,SATTM)                                                    03560686
      READ(5,VRATO)                                                    03560687
      READ(5,SUGCP)                                                    03560688
      READ(5,SUGBPE)                                                   03560689
      WRITE(6,DDPAN)                                                   03560690
      WRITE(6,PHYSP)                                                   03560691
      WRITE(6,LOADV)                                                   03560692
      WRITE(6,INTIAL)                                                  03560693
      WRITE(6,STABLE)                                                  03560694
C                                                                      03560695
      ILEFM1=ILEFT-1                                                   03560696
      ILEFP1=ILEFT+1                                                   03560697
      IDWNP1=IDOWN+1                                                   03560698
      IDOWM1=IDOWN-1                                                   03560699
      IRIGP1=IRIGHT+1                                                  03560700
      IF(IRIGHT.EQ.IMAX) IRIGP1=IMAX                                   03560701
      IMAXP1=IMAX+1                                                    03560702
      IMAXM1=IMAX-1                                                    03560703
      IMAXM2=IMAX-2                                                    03560704
      NCALM1=NCAL-1                                                    03560705
      NCALP1=NCAL+1                                                    03560706
      JMAXM1=JMAX-1                                                    03560707
      JMAXM2=JMAX-2                                                    03560708
      JMAXP1=JMAX+1                                                    03560709
      JMAXP2=JMAX+2                                                    03560710
C                                                                      03560711
      IF(STMODE.EQ.1) GO TO 6000                                       03560712
      TCONST = DSQRT(HMAX/GR)                                          03560713
      RATCR  = RATCR*TCONST/3600.0                                     03560714
      DIMPRS = DENSTY*HMAX/144.0D0                                     03560715
      PRESRF = PRESRF/DIMPRS                                           03560716
      DIMVIS = DENSTY*HMAX*DSQRT(HMAX*GR)/6.72E-04                     03560717
      CALL PARMEQ                                                      03560718
      B      = XIP(MN)+XSP(MN)                                         03560719
```

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      BPE    = BOILPE( XIP(MN) , XWP(MN) , B )*BETA                    03560720
      CONST1 = 1.0D0-XCP(MN)                                           03560721
      CONST2 = XCP(MN)/RHOC*DENSTY                                     03560722
      BB     = B/CONST1                                                03560723
      DELRH  = DELDDB*(BB-BRIXR)                                       03560724
      CP     = HEATC( XCP(MN) , BB)                                    03560725
 6000 CONTINUE                                                         03560726
      RHOVR  = RHOVR/DENSTY                                            03560727
      TSTEAM = (TSTEAM-TZERO)*BETA                                     03560728
      TINTAL = (TINTAL-TZERO)*BETA                                     03560729
C                                                                      03560730
      IF(STMODE.NE.1) GO TO 999                                        03560731
C                                                                      03560732
C     CALCULATE HEAT TRANSFER AREA AND NO. TUBES                       03560733
C                                                                      03560734
      TUBED  = TUBED/12.0D0                                            03560735
      A      = WVOL*AHTOV                                              03560736
      COMP2  = TUBED*TUBED/4.0D0*PIE                                   03560737
      COMP3  = TUBED*TUBEH*PIE                                         03560738
      NTUBES = A/COMP3                                                 03560739
      AREAT  = NTUBES*COMP3                                            03560740
      VOLSCH = NTUBES*COMP2*TUBEH                                      03560741
      DELR   = RAD/DFLOAT(IMAXM1)                                      03560742
      RIDWN  = DFLOAT(IDOWM1)*DELR                                     03560743
      VOLDWN = RIDWN**2*TUBEH*PIE                                      03560744
      BOTTH  = (WVOL-VOLSCH-VOLDWN)/RAD/RAD/PIE-WHEIG                  03560745
      HMAX   = BOTTH+TUBEH+WHEIG                                       03560746
      H      = PRECMX*HMAX                                             03560747
      POA    = AREAT/VOLSCH                                            03560748
      RADSQ  = RAD*RAD*PIE                                             03560749
C                                                                      03560750
      DR     = RAD/HMAX/DFLOAT(IMAXM1)                                 03560751
      DZ     = 1.0D0/DFLOAT(JJMAX)                                     03560752
      CDZ    = TUBEH/DFLOAT(NCALM1)/HMAX                               03560753
C                                                                      03560754
      TUBEH  = TUBEH/HMAX                                              03560755
```

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      TUBED  = TUBED/HMAX                                              03560756
      BOTTH  = BOTTH/HMAX                                              03560757
      CALANH = (TUBEH+BOTTH)*HMAX                                      03560758
      TCONST = DSQRT(HMAX/GR)                                          03560759
      RATCR  = RATCR*TCONST/3600.0D0                                   03560760
      DIMPRS = DENSTY*HMAX/144.0D0                                     03560761
      PRESRF = PRESRF/DIMPRS                                           03560762
      DIMVIS = DENSTY*HMAX*DSQRT(HMAX*GR)/6.72E-04                     03560763
      CALL PARMEQ                                                      03560764
      B      = XIP(MN)+XSP(MN)                                         03560765
      BPE    = BOILPE( XIP(MN) , XWP(MN) , B )*BETA                    03560766
      CONST1 = 1.0D0-XCP(MN)                                           03560767
      CONST2 = XCP(MN)/RHOC*DENSTY                                     03560768
      BB     = B/CONST1                                                03560769
      DELRH  = DELDDB*(BB-BRIXR)                                       03560770
      CP     = HEATC( XCP(MN) , BB)                                    03560771
      DHNEW  = CP*TINTAL                                               03560772
      CALL CALDEN(DD,DHNEW,TNEW,XV,XL,0.0D0,XVLIM)                     03560773
      RHO=DD                                                           03560774
      DH=H-CALANH                                                      03560775
      DH=DH/HMAX                                                       03560776
      JMAX=DH/DZ-2                                                     03560777
C*****************************************************                03560778
      IF(JMAX.GT.2)  GO TO 5122                                        03560779
      WRITE(6,1009)                                                    03560780
      STOP 53                                                          03560781
 1009 FORMAT(1X,'TRY AGAIN - NOT ENOUGH GRID POINTS')                  03560782
 5122 IF(JMAX.LT.29)  GO TO 5123                                       03560783
      WRITE(6,1010)                                                    03560784
      STOP 54                                                          03560785
 1010 FORMAT(1X,'TRY AGAIN - TOO MANY GRID POINTS')                    03560786
C*****************************************************                03560787
 5123 JMAX=DH/DZ-2                                                     03560788
      JMAXP2=JMAX+2                                                    03560789
      JMAXP1=JMAX+1                                                    03560790
      JMAXM1=JMAX-1                                                    03560791
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```
      JMAXM2=JMAX-2                                                    03560792
      SURFI=DH-JMAX*DZ                                                 03560793
      XXXX=0.0                                                         03560794
      S(MN)=XXXX                                                       03560795
      S(MO)=S(MN)                                                      03560796
      C(MN)=XXXX                                                       03560797
      C(MO)=C(MN)                                                      03560798
      IMP(MN)=XXXX                                                     03560799
      IMP(MO)=IMP(MN)                                                  03560800
      EM(MN)=XXXX                                                      03560801
      EM(MO)=EM(MN)                                                    03560802
      Q(MN)=XXXX                                                       03560803
      Q(MO)=Q(MN)                                                      03560804
      DO 5111 I=1,IMAX                                                 03560805
      FRAI(I)=XXXX                                                     03560806
      DHDT(I)=XXXX                                                     03560807
      W(MN,I,JMAXP2) = XXXX                                            03560808
      W(MO,I,JMAXP2) = XXXX                                            03560809
      DO 5111 J=1,JMAXP1                                               03560810
      U(MN,I,J)=XXXX                                                   03560811
      W(MN,I,J)=XXXX                                                   03560812
      DUDT(I,J)=XXXX                                                   03560813
      DEDT(I,J)=XXXX                                                   03560814
      DDDZDT(I,J)=XXXX                                                 03560815
      U(MO,I,J)=U(MN,I,J)                                              03560816
      W(MO,I,J)=W(MN,I,J)                                              03560817
      WW(I,J)=XXXX                                                     03560818
5111  CONTINUE                                                         03560819
      DO 5121 J=1,NCAL                                                 03560820
      HCDT(J)=XXXX                                                     03560821
      DDCDT(J)=XXXX                                                    03560822
      DO 5121 K=1,2                                                    03560823
      DO 5121 I=1,5                                                    03560824
5121  ZZZC(J,K,I)=XXXX                                                 03560825
      DO 52 I=1,IMAX                                                   03560826
```

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      P(I,JMAXP2)=0.0                                                  03560827
      P(I,JMAXP1)=0.5*SURFI*RHO                                        03560828
      P(I,JMAX)=SURFI*RHO                                              03560829
      SURFAC(I)=SURFI                                                  03560830
52    CONTINUE                                                         03560831
      SURFAC(IMAX+1)=SURFI                                             03560832
      DO 53 I=1,IMAX                                                   03560833
      DO 53 JJ=1,JMAXM1                                                03560834
      J=JMAX-JJ                                                        03560835
      JP1=J+1                                                          03560836
      P(I,J)=P(I,JP1)+DZ*RHO                                           03560837
53    CONTINUE                                                         03560838
      PBIP1=P(1,1)+TUBEH*RHO                                           03560839
      PBIM1=P(1,1)+TUBEH*RHO                                           03560840
      DO 533 I=1,IMAX                                                  03560841
      DO 533 J=1,JMAXP2                                                03560842
      T(MN,I,J)=TINTAL                                                 03560843
      DEN(MN,I,J)=RHO                                                  03560844
      ENTH(MN,I,J)=CP*TINTAL                                           03560845
      T(MO,I,J)=TINTAL                                                 03560846
      DEN(MO,I,J)=RHO                                                  03560847
      ENTH(MO,I,J)=CP*TINTAL                                           03560848
533   CONTINUE                                                         03560849
      AVERT(MN)=TINTAL                                                 03560850
      AVERT(MO)=AVERT(MN)                                              03560851
      AVERH(MN)=CP*TINTAL                                              03560852
      AVERH(MO)=AVERH(MN)                                              03560853
      AVERD(MN)=RHO                                                    03560854
      AVERD(MO)=AVERD(MN)                                              03560855
      TDWNJP(MN)=TINTAL                                                03560856
      TBOTT(MN)=TINTAL                                                 03560857
      TCALJM(MN)=TINTAL                                                03560858
      TCALAV(MN)=TINTAL                                                03560859
      DDWNJP(MN)=RHO                                                   03560860
      DBOTT(MN)=RHO                                                    03560861
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DCALJM(MN)=RHO                                                  03560862
DCALAV(MN)=RHO                                                  03560863
HDWNJP(MN)=CP*TINTAL                                            03560864
HBOTT(MN)=CP*TINTAL                                             03560865
HCALJM(MN)=CP*TINTAL                                            03560866
HCALAV(MN)=CP*TINTAL                                            03560867
TDWNJP(MO)=TINTAL                                               03560868
TBOTT(MO)=TINTAL                                                03560869
TCALJM(MO)=TINTAL                                               03560870
TCALAV(MO)=TINTAL                                               03560871
DDWNJP(MO)=RHO                                                  03560872
DBOTT(MO)=RHO                                                   03560873
DCALJM(MO)=RHO                                                  03560874
DCALAV(MO)=RHO                                                  03560875
HDWNJP(MO)=CP*TINTAL                                            03560876
HBOTT(MO)=CP*TINTAL                                             03560877
HCALJM(MO)=CP*TINTAL                                            03560878
HCALAV(MO)=CP*TINTAL                                            03560879
WCALAV(MN)=0.0                                                  03560880
WCALAV(MO)=0.0                                                  03560881
WDWNJP(MN)=0.0                                                  03560882
WDWNJP(MO)=0.0                                                  03560883
WDWNJM(MN)=0.0                                                  03560884
WDWNJM(MO)=0.0                                                  03560885
WCALJM(MN)=0.0                                                  03560886
WCALJM(MO)=0.0                                                  03560887
UBOTT(MN)=0.0                                                   03570000
UBOTT(MO)=0.0                                                   03580000
HHM(MN)=H                                                       03590000
HHM(MO)=HHM(MN)                                                 03600000
HH(MN)=H                                                        03610000
HH(MO)=HH(MN)                                                   03620000
VOLC=VOLSCH+BOTTH*HMAX*RADSQ+VOLDWN                             03630000
DH=HHM(MN)-CALANH                                               03640000
VOLP=VOLC+DH*RADSQ                                              03650000
TMASS(MN)=DENSTY*AVERD(MN)*VOLP                                 03660000
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      TOTALH(MN)=TMASS(MN)*AVERH(MN)                                    03670000
      TOTALH(MO)=TOTALH(MN)                                             03680000
      WATER(MN)=XWP(MN)*TMASS(MN)                                       03690000
      S(MN)=XSP(MN)*TMASS(MN)                                           03700000
      IMP(MN)=XIP(MN)*TMASS(MN)                                         03710000
      C(MN)=XCP(MN)*TMASS(MN)                                           03720000
      WATER(MO)=WATER(MN)                                               03730000
      S(MO)=S(MN)                                                       03740000
      IMP(MO)=IMP(MN)                                                   03750000
      C(MO)=C(MN)                                                       03760000
      TMASS(MO)=TMASS(MN)                                               03770000
      SS      = SUPERS(AVERT(MN),XSP(MN),XIP(MN),XWP(MN))               03780000
      G(MN)   = GROWTH(AVERT(MN),SS,XIP(MN),XWP(MN))                    03790000
      G(MO)   = G(MN)                                                   03800000
      DO 5331 J=1,NCAL                                                  03810000
      CALT(J,MN)=TINTAL                                                 03820000
      CALH(J,MN)=TINTAL*CP                                              03830000
      CALD(J,MN)=RHO                                                    03840000
      CALT(J,MO)=TINTAL                                                 03850000
      CALH(J,MO)=TINTAL*CP                                              03860000
      CALD(J,MO)=RHO                                                    03870000
      CALW(J,MN)=0.0                                                    03880000
      CALW(J,MO)=0.0                                                    03890000
 5331 CONTINUE                                                          03900000
      CALP(NCAL,MN)=P(1,1)                                              03910000
      CALP(NCAL,MO)=P(1,1)                                              03920000
      DO 5332 JJ=1,NCALM1                                               03930000
      J=NCAL-JJ                                                         03940000
      CALP(J,MN)=CALP(J+1,MN)+CDZ*RHO                                   03950000
      CALP(J,MO)=CALP(J,MN)                                             03960000
 5332 CONTINUE                                                          03970000
C                                                                       03980000
  999 CONTINUE                                                          03990000
C                                                                       04000000
      UU      = UU*TCONST/3600.0D0                                      04010011
```

```
      UA      = UU*AREAT                                                  04020000
      UPOA    = POA*UU/DENSTY                                             04030000
      DIMKV   = HMAX*DSQRT(HMAX*GR)                                       04040001
      VART    = VART/DIMKV                                                04050001
      SFSMTH  = SFSMTH/DIMKV                                              04060001
      ALPHA   = ALPHA/DIMKV                                               04070001
      R(1)    = 0.0                                                       04080000
      R(2)    = 0.5D0*DR                                                  04090000
      RH(1)   = 0.0                                                       04100000
      RH(2)   = DR                                                        04110000
      DO 100 I=3,IMAX                                                     04120000
      IM1=I-1                                                             04130000
      R(I)    = R(IM1)+DR                                                 04140000
      RH(I)   = RH(IM1)+DR                                                04150000
  100 CONTINUE                                                            04160000
      R(IMAX+1)=0.0                                                       04170000
      DO 3 I=2,IMAX                                                       04180000
      RI      = R(I)                                                      04190000
      RINV(I)=1.0D0/RI                                                    04200000
      RIP1    = RI+DR*0.5D0                                               04210000
      RIM1    = RI-DR*0.5D0                                               04220000
      DV(I)   = RIP1*RIP1-RIM1*RIM1                                       04230000
    3 CONTINUE                                                            04240000
      RINV(1)= 9.99E+70                                                   04250000
      DV(1)   = 9.99E+70                                                  04260000
      COMP1   = (R(IMAX)+0.5D0*DR)*(R(IMAX)+0.5D0*DR)                     04270000
      DO  5 I=1,IMAX                                                      04280000
      DVOA(I)= DV(I)/COMP1                                                04290000
    5 CONTINUE                                                            04300000
      Z(1)   = 0.0                                                        04310000
      DO 2 J=2,JMAXP1                                                     04320000
    2 Z(J)   = Z(J-1)+DZ                                                  04330000
      DRT2    = DR*2.0D0                                                  04340000
      SLIPV   = SLIPV/DSQRT(GR*HMAX)                                      04350000
      DTOTH   = DT/TUBEH                                                  04360000
      THODT   = TUBEH/DT                                                  04370000
```

```
      DTOCDZ = DT/CDZ                                                  04380000
      FOURMC = DTOCDZ/CDZ*ALPHA                                        04390000
      DTO2DR = DT/(2.0D0*DR)                                           04400000
      DTODR  = DT/DR                                                   04410000
      FOURMR = DT*ALPHA/DR**2                                          04420000
      DTORSQ = DT/(DR*DR)                                              04430000
      FMO2DR = DT*ALPHA/DR*0.5D0                                       04440000
      FMODR  = DTODR*ALPHA                                             04450000
      FMO2DR = DTO2DR*ALPHA                                            04460000
C                                                                      04470000
      CALL SETUPP                                                      04480000
      CALL INCONV                                                      04490000
C                                                                      04500000
      RIP1   = R(IRIGHT)+0.5D0*DR                                      04510000
      RIM1   = R(ILEFT)-0.5D0*DR                                       04520000
      COMP2  = RIP1*RIP1-RIM1*RIM1                                     04530000
      FMOM   = COMP2/(DFLOAT(NTUBES)*TUBED**2/4.0D0)                   04540000
      VOLUP  = VOLSCH/PIE/HMAX**3                                      04550000
      AFLWD  = R(IDOWN)+0.5D0*DR                                       04560000
      AFLWD  = AFLWD*AFLWD                                             04570000
      RIM1   = R(ILEFT)-0.5D0*DR                                       04580000
      RIP1   = R(IRIGHT)+0.5D0*DR                                      04590000
      AFLWU  = RIP1*RIP1-RIM1*RIM1                                     04600000
      COMP2  = 2.0D0*BOTTH*(R(IDOWN)+0.5D0*DR)                         04610000
      ABOAFD = COMP2/AFLWD                                             04620000
      ABOAFU = COMP2/AFLWU                                             04630000
      RIM1   = R(IDOWN)+0.5D0*DR                                       04640000
      V1     = AFLWD*TUBEH+BOTTH*RIM1*RIM1                             04650000
      RIP1   = R(IMAX)+0.5D0*DR                                        04660000
      V2     = BOTTH*(RIP1*RIP1-RIM1*RIM1)                             04670000
      VOLET  = V1+V2                                                   04680000
      DTAUOV = DT*AFLWU/VOLBT                                          04690000
      F      = F*ICONST/3600.0D0                                       04700011
      XIF    = BRIXFF*(1.0-PURFF)                                      04710000
      XSF    = BRIXFF*PURFF                                            04720000
```

```
      XWF     = 1.0-XSF-XIF                                              04730000
      HF      = HEATC(0.0D0,BRIXFF)*(TEMPFF-TZERO)                       04740000
C                                                                        04750000
C                                                                        04760000
      RIP1    = R(ILEFT)-0.5D0*DR                                        04770000
      RIM1    = R(IDOWN)+0.5D0*DR                                        04780000
      RAV     = (RIP1+RIM1)/2.0D0                                        04790000
      DELTAR  = RIP1-RIM1                                                04800000
      DELRSQ  = RIP1*RIP1-RIM1*RIM1                                      04810000
      DNVR    = 1.0D0/RIP1-1.0D0/RIM1                                    04820000
      IF(DELTAR.LE.0.0) STOP 60                                          04830000
C     CONST8 = -(1.0D0/RIP1)**3*RAV LIMITING VALUE                       04840000
C     GO TO 2222                                                         04850000
      CONST8 = 2.0D0*DNVR/DELRSQ*RAV**2                                  04860000
      CONST6 = RAV/RIM1                                                  04870000
      CONST7 = 1.0D0/DELTAR                                              04880000
      HHH(MN)=HH(MN)                                                     04890000
      HHH(MO)=HH(MN)                                                     04900000
      HHM(MN)=HH(MN)                                                     04910000
      HHM(MO)=HH(MO)                                                     04920000
C------- INTIALIZE VARIABLES THAT ARE CONTRAINTED BY CONTROL --          04930009
C------- OR BY MATERIAL AND ENERGY BALANCES ------------------           04940009
      CALL ECNTRL                                                        04950010
      CALL CONTRL                                                        04960009
C-----------------------------------------------------------------       04970009
      BB      = (XIP(MN) + XSP(MN))/CONST1                               04980009
      V       = CONST2*AVERD(MN)/(1.0D0-CONST2*AVERD(MN))                04990000
      VRATIO  = RATIO( V , AVERLL(MN) )                                  05000000
      VORHO   = VKINEM(AVERT(MN),BB)                                     05010000
      HVAP    = ENTHV(0.0D0,0.0D0,BPE)                                   05020000
C----- INTIALIZE HEAT FLUX ACCORDING TO PROBLEM -----                   05030009
      CALL INHEAT(EVAP)                                                  05040013
      CALL HEATIN( CALT, QFLUX, AQFLUX )                                 05050008
C-----------------------------------------------------------------       05060009
```

```
      DO 2225 I=2,IMAX                                                  05070000
2225  SSURF(I)=SURFAC(I)                                                05080000
      DO 2226 J=1,JMAX                                                  05090000
      JJJ=2*J-1                                                         05100000
2226  DPDT(J)=DDZDT*DFLOAT(JJJ)*0.5D0                                   05110000
1002  FORMAT(1X,6I6)                                                    05180000
      RETURN                                                            05190000
      END                                                               05200000
```

```
      SUBROUTINE PRES                                                    05200003
C-----                                                                   05200004
C-----   MOTIVE SUBROUTINE FOR PRESSURE CALCULATION IN                   05200005
C-----   PAN PROPER                                                      05200006
C-----                                                                   05200007
      IMPLICIT REAL*8(A-H,O-Z)                                           05200008
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA               05200009
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 05200010
     2,             HVINV,DELHLV,DENSTY                                 05200011
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                           05200012
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT    05200013
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1              05200014
      COMMON/STEP/MN,MO,N                                                05200015
      COMMON/SIZE/H,RAD,HMAX                                             05200016
      COMMON /AREAP/DV(30),DVOA(30)                                      05200017
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN               05200018
     1,IDWNP1,IDOWM1                                                     05200019
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                    05200020
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                05200021
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                 05200022
      COMMON/IPHASE/ENTH(2,30,30),DEN(2,30,30)                           05200023
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODP,DZO2DR,DTO2DR,DTO2DZ       05200024
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                    05200025
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                   05200026
     3,             DZODTO                                              05200027
C                                                                        05200028
      DO 60 I=2,IMAX                                                     05200029
      SURFI=0.5D0*SURFAC(I)                                              05200030
      DJP1=DEN(MN,I,JMAXP1)                                              05200031
      DNEW=DEN(MN,I,JMAX)                                                05200032
      P(I,JMAXP1)=SURFI*DJP1                                             05200033
      P(I,JMAX)=2.0D0*SURFI*DJP1+DZO2*DNEW                               05200034
      DO 60 JJ=1,JMAXM1                                                  05200035
      J=JMAX-JJ                                                          05200036
      JP1=J+1                                                            05200037
```

```
      DJP1=DNEW                                                    05200038
      DNEW=DEN(MN,I,J)                                             05200039
      P(I,J)=DZ02*(DNEW+DJP1)+P(I,JP1)                             05200040
60    CONTINUE                                                     05200041
      RETURN                                                       05200042
      END                                                          05200043
```

```
      SUBROUTINE PRESSC                                                      05200046
C-----                                                                       05200047
C-----  CALCULATION OF ONE-D PRESSURE PROFILE IN CALANDRIA                   05200048
C-----                                                                       05200049
      IMPLICIT REAL*8(A-H,O-Z)                                               05200050
      DIMENSION ZZZZ(2,20),ZZZC(10,2,5)                                      05200051
      REAL*8 IMP(2)                                                          05200052
      COMMON/CONC  /DELDDB,DELRH,BRIXR,CONST1,CONST2,BPE,VRATIO              05200053
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)            05200054
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                      05200055
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                        05200056
     3,             SSMAX, SSMIN                                            05200057
      COMMON/PAN/ VOLSCH, RADSQ, VCIC, WVCL, WHEIG                           05200058
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                     05200059
      COMMON/TPHASE/ENTH(2,30,30),DEN(2,30,30)                               05200060
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ           05200061
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                        05200062
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDI,DRT2,DZO,DDZDTO                       05200063
     3,             DZODTO                                                  05200064
      COMMON/PROPTY/RHO,RHOINV,RHOC2,VISC,ALPHA,VORHO,BETA                   05200065
     1,              FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                     05200066
     2,              HVINV,DELHLV,DENSTY                                     05200067
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                               05200068
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT        05200069
     1,             NBAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1                  05200070
      COMMON/STEP/MN,MC,N                                                    05200071
      COMMON/SIZE/H,RAD,HMAX                                                 05200072
      COMMON /AREAP/DV(30),DVOA(30)                                          05200073
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILEFP1,ILEFM1,IDOWN                   05200074
     1,IDWNP1,IDOWM1                                                         05200075
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH        05200076
     1,BOTTH,TUBED,FMCM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                 05200077
     2,NCALP1                                                                05200078
      COMMON/LUMBT/WDWNJP(2),TDWNJP(2),DDWNJP(2),HDWNJP(2)                   05200079
     1,WDWNJH(2),TBOTT(2),DBOTT(2),HBOTT(2)                                  05200080
```

```
     2,UBOTT(2),UONEB(2),WCALAV(2),TCALAV(2),DCALAV(2),HCALAV(2)          05200081
     3,WCALJM(2),TCALJM(2),DCALJM(2),HCALJM(2)                           05200082
      COMMON/LUMCAL/ CALW(10,2),CALH(10,2),CALT(10,2),CALD(10,2)         05200083
     1,CALP(10,2)                                                        05200084
      DATA PIE,COEFFV,RHOC,GR/3.14159D0,0.5236D0,99.1D0,32.2D0/          05200085
      EQUIVALENCE (ZZZZ,WDWNJP)                                          05200086
      EQUIVALENCE (ZZZC,CALW)                                            05200087
C                                                                        05200088
C-------- CALCULATE PRESSURE AT TOP OF CALANDRIA ---                     05200089
C                                                                        05200090
      PNUP=0.0                                                           05200091
      COMP1=0.0                                                          05200092
      DO 63 I=ILEFT,IRIGHT                                               05200093
      DDVI=DV(I)                                                         05200094
      PNUP=PNUP+DDVI*(P(I,1)+DZO2*DEN(MN,I,1))                           05200095
      COMP1=COMP1+DDVI                                                   05200096
 63   CONTINUE                                                           05200097
      PNUP=PNUP/COMP1                                                    05200098
C                                                                        05200099
C-------- CALCULATE PRESSURE PROFILE IN CALANDRIA                        05200100
C                                                                        05200101
      CALP(NCAL,MN)=PNUP                                                 05200102
      CALL CALPP(PBIP1)                                                  05200103
C                                                                        05200104
C-------- CALCULATE PRESSURE AT TOP OF DOWNTAKE                          05200105
C                                                                        05200106
      PNUP=0.0                                                           05200107
      COMP1=0.0                                                          05200108
      DO 61 I=2,IDOWN                                                    05200109
      DDVI=DV(I)                                                         05200110
      PNUP=PNUP+DDVI*(P(I,1)+DZO2*DEN(MN,I,1))                           05200111
      COMP1=COMP1+DDVI                                                   05200112
 61   CONTINUE                                                           05200113
      PNUP=PNUP/COMP1                                                    05200114
C                                                                        05200115
C---------- CALCULATE PRESSURE AT BOTTOM OF DOWNTAKE ----               05200116
```

```
      B    = (XSP(MN) + XIP(MN))/(1.0D0 - XCP(MN) )                    05200118
      DNEW=DBCTT(MN)                                                   05200119
      WAV=WDWNJM(MN)+WDWNJM(MO)                                        05200120
      RIP1=R(IDOWN)+0.5D0*DR                                           05200121
      DPFR=4.0D0*TUBEH*VISCTY(TBOTT(MN),B)*WAV/RIP1/RIP1*VRATIO        05200122
C                                                                      05200123
CC                                                                     05200124
      PBIM1=PNUP+DNEW*TUBEH+DPFR                                       05200125
C                                                                      05200126
CC                                                                     05200127
      RETURN                                                           05200128
      END                                                              05200129
                                                                       05200130
```

```
      SUBROUTINE REZONE
C-----                                                                  05200133
C----    CALCULATIONS FOR DYNAMIC GRID                                  05200134
C-----                                                                  05200135
      IMPLICIT REAL*8(A-H,O-Z)                                          05200136
      REAL*8 IMP(2)                                                     05200137
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),dH(2)       05200138
     1,            F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)     05200139
     2,            TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)       05200140
     3,            SSMAX, SSMIN                                         05200141
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX               05200142
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                      05200143
      COMMON/MOVE   / DPDT(30)                                          05200144
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                   05200145
     1,          SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                05200146
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      05200147
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZOBSQ,DZODT,DTORSQ                   05200148
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  05200149
     3,            DZODTO                                              05200150
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              05200151
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 05200152
     2,             HVINV,DELHLV,DENSTY                                 05200153
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          05200154
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   05200155
     1,             NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1             05200156
      COMMON/STEP/MN,MO,N                                               05200157
      COMMON/SIZE/H,RAD,HMAX                                            05200158
      COMMON /AREAP/DV(30),DVOA(30)                                     05200159
      COMMON/BOUND/IRIGHT,IRIGP1,ILEFT,ILFTP1,ILEFM1,IDOWN              05200160
     1,IDWNP1,IDOWM1                                                    05200161
C                                                                       05200162
      SURFDT=(HH(MO)-HH(MN))/DT                                         05200163
      DDZDTO=DDZDT                                                      05200164
      DDZDT=(SURFDT/DFLOAT(JMAX)/HMAX-DDZDT)*THETAZ+DDZDT               05200165
      CALL SETUP                                                        05200166
```

```
      DO 8555 J=1,JMAX                                                  05200167
      JJJ=2*J-1                                                         05200168
8555  DPDT(J)=DDZDT*DFLOAT(JJJ)*0.5D0                                   05200169
      RETURN                                                            05200170
      END                                                               05200171
                                                                        05200172
```

```
      SUBROUTINE RMOMEQ
C-----                                                                  05200175
C-----   INTEGRATION RADIAL MOMENTUM EAN PROPER                         05200176
C-----                                                                  05200177
      IMPLICIT REAL*8(A-H,O-Z)                                          05200178
      COMMON/DIMEM/U(2,30,30),W(2,30,30),T(2,30,30),WW(30,30)           05200179
      COMMON/DIMEN1/P(30,30),PBIP1,PBIM1                                05200180
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      05200181
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   05200182
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DDZO,DDZDTO                 05200183
     3,           DZODTO                                               05200184
      COMMON/PROPTY/RHO,RHOINV,RHCC2,VISC,ALPHA,VORHO,BETA              05200185
     1,            FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                 05200186
     2,            HVINV,DELHLV,DENSTY                                 05200187
      COMMON/COORD/R(30),Z(30),RINV(30),RH(30)                          05200188
      COMMON/LIMITS/IMAX,IMAXM1,IMAXM2,JMAX,JMAXM1,JMAXM2,NMAX,NPRINT   05200189
     1,            NEAR,NPRNT,JMAXP1,NSTART,JMAXP2,IMAXP1              05200190
      COMMON/STEP/MN,MO,N                                               05200191
      COMMON/TEMP/TNEW,TOLD,TIP1,TIM1,TJP1,TJM1                         05200192
      COMMON/CONSER/DIP1,DIM1,DJP1,DJM1,RIP1,RIM1,RI,RHIP1,RHIM1        05200193
     1,ADIP1,ADIM1,ADJP1,ADJM1                                          05200194
      COMMON/VELCTY/UNEW,UOLD,WNEW,WOLD,UIP1,UIM1,UJP1,UJM1,WIP1,WIM1   05200195
     1,WJP1,WJM1,UF,UB,WF,WB                                            05200196
      COMMON/PRESS/PIP1,PIM1,PJ,PJP1                                    05200197
      COMMON/INDEX/I,J                                                  05200198
      COMMON/FLOW1/DUDT(30,30),DEDT(30,30),HCDT(10),BTDUDT,BTDEDT       05200199
     1,DDDZDT(30,30),DDCDT(10)                                          05200200
      COMMON/SUBDER/DPDTI                                               05200201
C                                                                       05200202
      UUF=0.0                                                           05200203
      IF(UF.LT.0.0)  UUF=UIP1-UOLD                                      05200204
      UUB=UIM1-UOLD                                                     05200205
      IF(UB.LT.0.0)  UUB=0.0                                            05200206
      UWF=0.0                                                           05200207
      IF(WF.LT.0.0)  UWF=UJP1-UOLD                                      05200208
```

```
      UWB=UJM1-UOLD                                                     05200209
      IF(WB.LT.0.0)  UWB=0.0                                            05200210
C                                                                       05200211
C                                                                       05200212
C                                                                       05200213
C                                                                       05200214
      COMP1=DTO2DR*RINV(I)*(UF*UUF-UB*UUF)                              05200215
      COMP2=DTODZ*(WF*UWF-WB*UWB)                                       05200216
      COMP3=VORHO*DTORSQ*RINV(I)*(RHIP1*(UIP1-UOLD)*ALIP1              05200217
     1-RHIM1*(UOLD-UIM1)*ADIM1)                                         05200218
      COMP5=VORHO*DTOZSQ*(ADJP1*(UJP1-UOLD)-ADJM1*(UOLD-UJM1))          05200219
      COMP6=DTO2DR*(PIM1-PIP1)                                          05200220
      COMP7=-VORHO*DT*RINV(I)*RINV(I)*UOLD                              05200221
      DUODT=(-COMP1-COMP2+COMP3+COMP5+COMP6)*RHOINV+COMP7               05200222
      UNEW=UOLD+(DUDT(I,J)*DT+DUODT)*0.5D0                              05200223
      DUDT(I,J)=DUODT/DT                                                05200224
      RETURN                                                            05200225
      END                                                               05200226
```

```
      SUBROUTINE SETUP                                                  05200229
C-----                                                                  05200230
C-----  CALCULATION OF NEW GRID CONSTANTS (DZ)                          05200231
C-----                                                                  05200232
      IMPLICIT REAL*8(A-H,O-Z)                                          05200233
      COMMON/GRID/DR,DZ,DT,DTO2SQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ      05200234
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                   05200235
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                  05200236
     3,             DZODTO                                             05200237
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA              05200238
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                05200239
     2,             HVINV,DELHLV,DENSTY                                05200240
      COMMON/CHEST/UU,UA,TUBEH,AREAT,FOA,UFOA,DTOTH,THODT,UAOA,CALANH   05200241
     1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1            05200242
     2,NCALP1                                                           05200243
C                                                                       05200244
      DZO=DZ                                                            05200245
      DZODTO=DZODT                                                      05200246
      DZ=DZO+DDZDT*DT                                                   05200247
      ENTRY SETUPP                                                      05200248
      CALFC2=(DZ+CDZ)*0.5D0                                             05200249
      DZO2=DZ/2.0D0                                                     05200250
      DTO2SQ=DT/DZ**2                                                   05200251
      DTODZ=DT/DZ                                                       05200252
      DZODR=DZ/DR                                                       05200253
      DZO2DR=DZ/(2.0D0*DR)                                              05200254
      DZORSQ=DZ/DR**2                                                   05200255
      DZODT=DZ/DT                                                       05200256
      DTO2DZ=DT/(2.0D0*DZ)                                              05200257
      DT2DRZ=DT/(2.0D0*DR*DZ)                                           05200258
      DTODRZ=DT/(DR*DZ)                                                 05200259
      FOURMD=DT*ALPHA/DZ**2                                             05200260
      RETURN                                                            05200261
      END
```

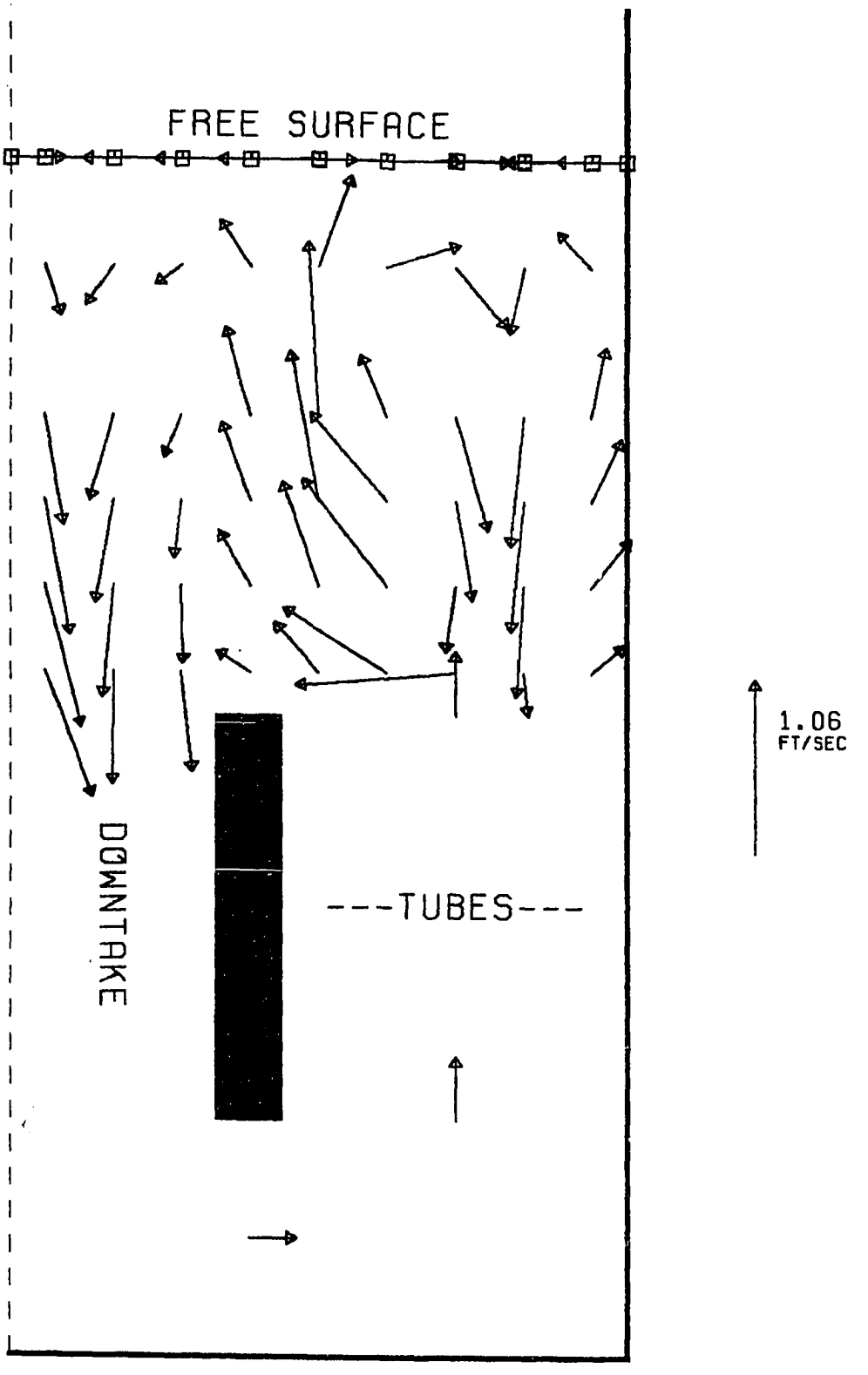
```
      SUBROUTINE WMIXT                                                      05200264
C----                                                                       05200265
C----  WELL MIX TANK CALCULATIONS.                                          05200266
C----  OVERALL MATERIAL BALANCES, CRYSTAL GROWTH.                           05200267
C---- CALCULATION OF PERTINENT AVERAGE PHYSICAL PROPERTIES                  05200268
C---- (VISCOSITY).                                                          05200269
C----                                                                       05200270
      IMPLICIT REAL*8(A-I,O-Z)                                              05200271
      REAL*8 IMP(2)                                                         05200272
      COMMON/TOP/ SURFAC(30),SSURF(30),SVFRV(30),HVAP                       05200273
     1,           SFSMTH,THETAZ,THETAS,FRAT(30),DHDT(30)                  05200274
      COMMON/CONC  /DELDDB,DELBH,BRIXR,CONST1,CONST2,BPE,VRATIO             05200275
      COMMON/AVPART/AVERNN(2),AVERLL(2)                                     05200276
      COMMON/PROPTY/RHO,RHOINV,RHOO2,VISC,ALPHA,VORHO,BETA                  05200277
     1,             FOURMR,FMO2DR,FMODR,CP,FOURMC,TZERO                    05200278
     2,             HVINV,DELHLV,DENSTY                                    05200279
      COMMON/WSTRT/EM(2),S(2),IMP,C(2),Q(2),AVERT(2),HHM(2),HH(2)           05200280
     1,F,XWF,XSF,XIF,G(2),HF,AVERD(2),TMASS(2),WATER(2)                     05200281
     2,TOTALH(2),XSP(2),XIP(2),XCP(2),XWP(2),AVERH(2)                       05200282
     3,          SSMAX, SSMIN                                               05200283
      COMMON/OVERAL/ E(2), HHH(2), EVINTO, EMVINT, AQFLUX                   05200284
      COMMON/GRID/DR,DZ,DT,DTOZSQ,DTODZ,DZODR,DZO2DR,DTO2DR,DTO2DZ          05200285
     1,DT2DRZ,DTODRZ,DTODR,FOURMD,DZORSQ,DZODT,DTORSQ                       05200286
     2,DZO2,CALFC2,CALFC3,DDZDT,SURFDT,DRT2,DZO,DDZDTO                      05200287
     3,          DZODTO                                                     05200288
      COMMON/STEP/MN,MO,N                                                   05200289
      COMMON/PAN/ VOLSCH, RADSQ, VOLC, WVOL, WHEIG                          05200290
      COMMON/ENTHAL/DHNEW,DHOLD,DHIP1,DHIM1,DHJP1,DHJM1                     05200291
      COMMON/CHEST/UU,UA,TUBEH,AREAT,POA,UPOA,DTOTH,THODT,UAOA,CALANH       05200292
     1,BOTTH,TUBED,FMOM,CDZ,DTOCDZ,TSTEAM,NTUBES,NCAL,NCALM1                05200293
     2,NCALP1                                                               05200294
      COMMON/VAPDEN/PRESRF,RHOVR                                            05200295
      COMMON/ BLOCK  /  BRIXFF, PURFF,TEMPFF,                               05200296
     1      VART, PRECMX, AHTOV, HF, TINTAL, HV, JJMAX                      05200297
      DATA RHOC, COEFFV / 99.1D0, 0.5236D0 /                                05200298
C                                                                           05200299
                                                                            05200300
```

```
C                                                                       05200301
      AVERLL(MN) = AVERLL(MO) + (G(MN)+G(MO)) * DT*0.5D0                05200302
      IF(AVERLL(MN).LT.0.0) AVERLL(MN)=0.0                              05200303
      DELC  = (AVERLL(MN)**3-AVERLL(MO)**3)*RHOC*COEFFV*AVERNN(MN)      05200304
      WATER(MN)=WATER(MO) + (F*XWF- EM(MN)) *DT                         05200305
      S(MN)     =S(MO)     +  F*XSF*DT - DELC                           05200306
      IMP(MN)   =IMP(MO)   +  F*XIF*DT                                  05200307
      C(MN)     =C(MO)     +  DELC                                      05200308
      TMASS(MN)=TMASS(MO)+ (F   -   EM(MN) )*DT                         05200309
C                                                                       05200310
C     CALCULATION OF MASS FRACTION                                      05200311
C                                                                       05200312
      COMP1=TMASS(MN)                                                   05200313
      COMP2=S(MN)/COMP1                                                 05200314
      COMP3=IMP(MN)/CCMP1                                               05200315
      COMP4=C(MN)/COMP1                                                 05200316
      COMP5=WATER(MN)/COMP1                                             05200317
      SUM=COMP2+COMP3+COMP4+COMP5                                       05200318
      XSP(MN)=COMP2/SUM                                                 05200319
      XIP(MN)=COMP3/SUM                                                 05200320
      XCP(MN)=COMP4/SUM                                                 05200321
      XWP(MN)=COMP5/SUM                                                 05200322
C                                                                       05200323
C     CALCULATION AVERAGE PAN HEIGHT                                    05200324
C                                                                       05200325
      VOLP=TMASS(MN)/DENSTY/AVERD(MN)                                   05200326
      VOLP=VOLP-VOLC                                                    05200327
      HHM(MN)=VOLP/RADSQ+CALAWH                                         05200328
C                                                                       05200329
C     CALCULATION AVERAGE PROPERTY                                      05200330
C                                                                       05200331
      B=XIP(MN)+XSP(MN)                                                 05200332
      BPE    = BOILPE( XIP(MN) , XWP(MN) , B )*BETA                     05200333
      CONST1 = 1.0D0-XCP(MN)                                            05200334
      CONST2 = XCP(MN)/RHOC*DENSTY                                      05200335
```

```
      BB=B/CONST1                                                       05200336
      CP      = HEATC( XCP(MN) , BB )                                   05200337
      DELRH   = DELDDB*(BB-BRIXR)                                       05200338
      V=CONST2*AVERD(MN)/(1.0D0-CONST2*AVERD(MN))                       05200339
      VRATIO = RATIO( V , AVERLL(MN) )                                  05200340
      VORHO   = VKINEM(AVERT(MN),BB)                                    05200341
      HVAP    = ENTHV(0.0D0,0.0D0,BPE)                                  05200342
C                                                                       05200343
      RETURN                                                            05200344
      END                                                               05200345
```

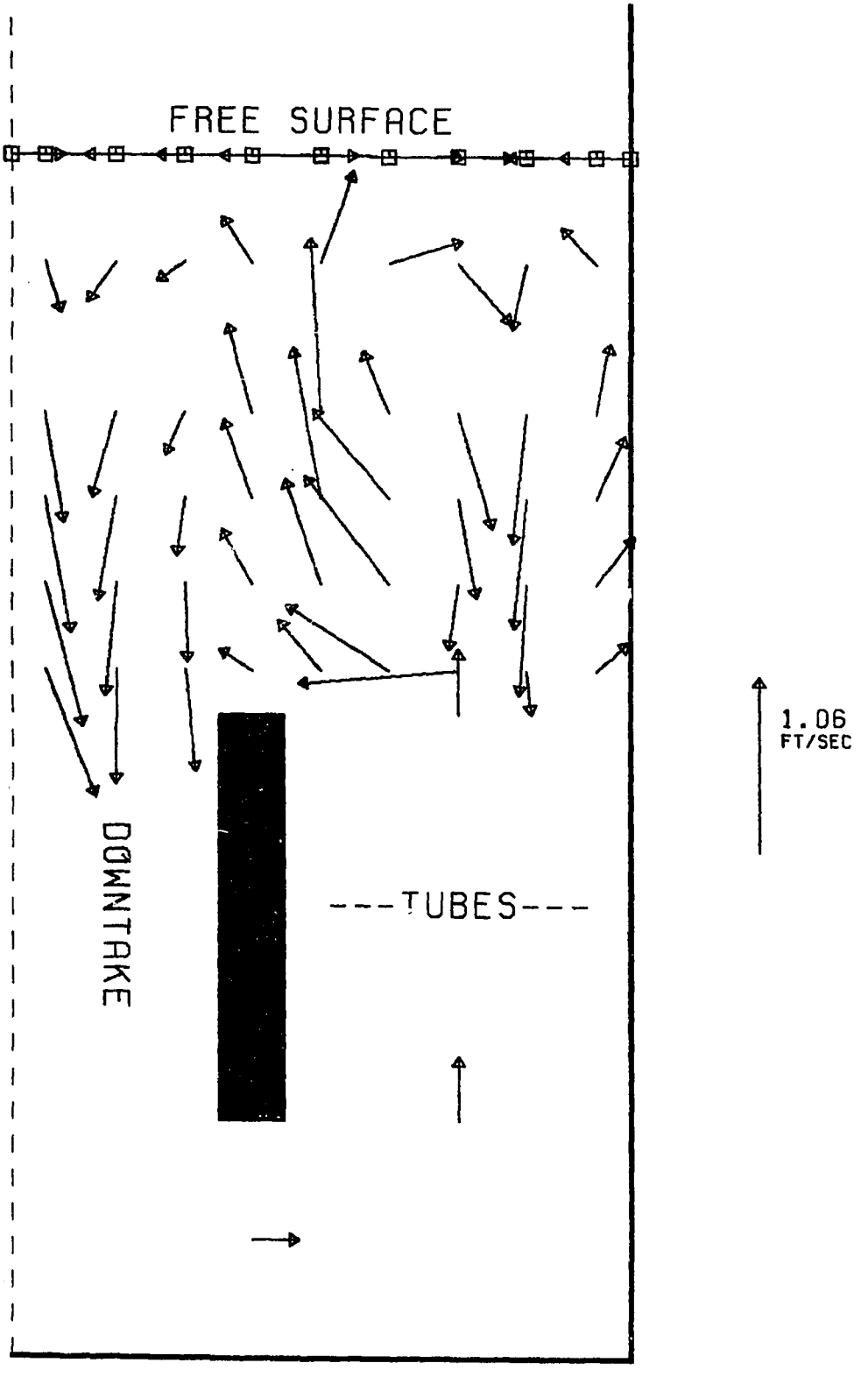
APPENDIX II

EFFECT OF THERMAL DIFFUSIVITY AND KINEMATIC VISCOSITY



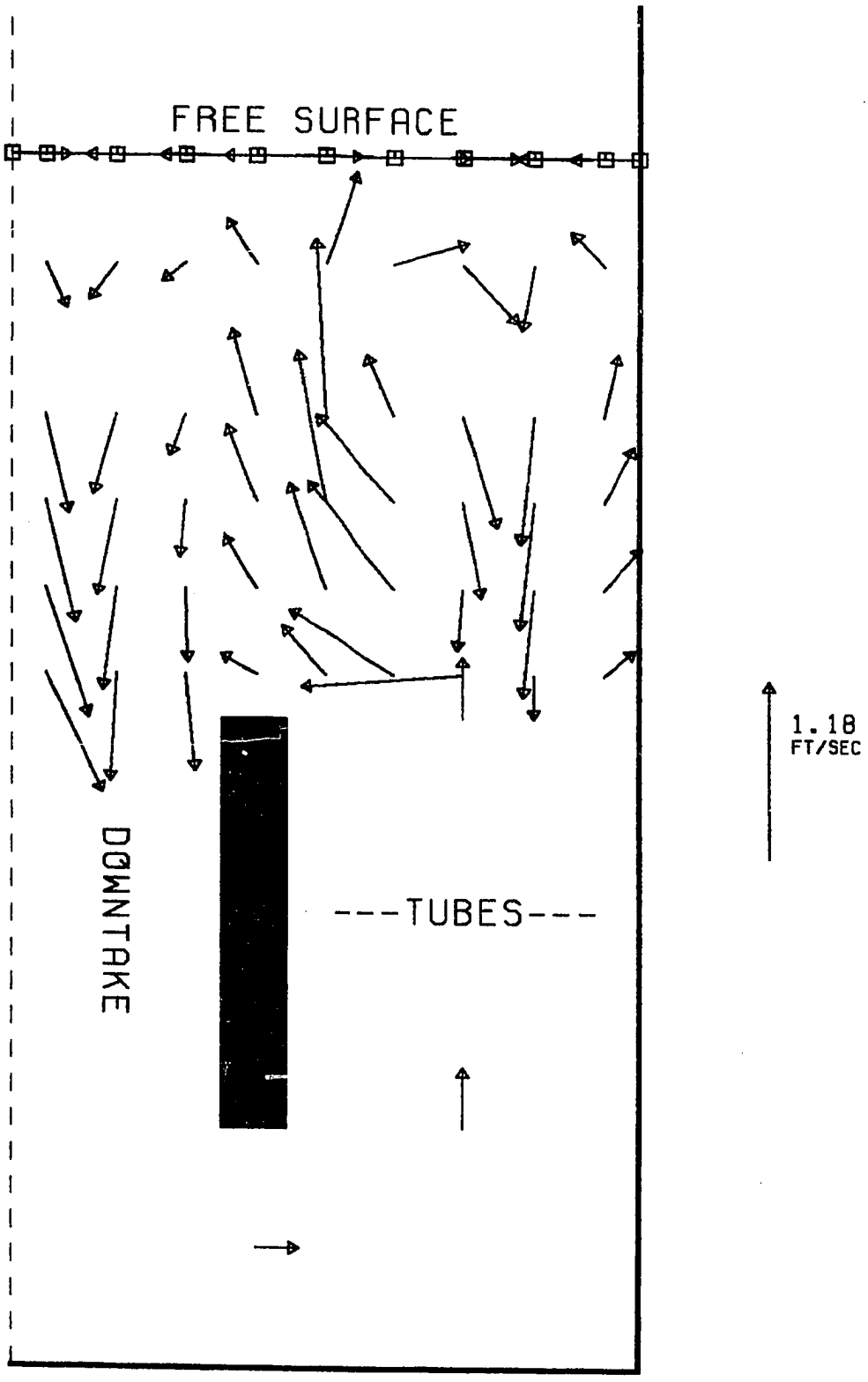
VELOCITY VECTORS

FIGURE II.1 CASE 1



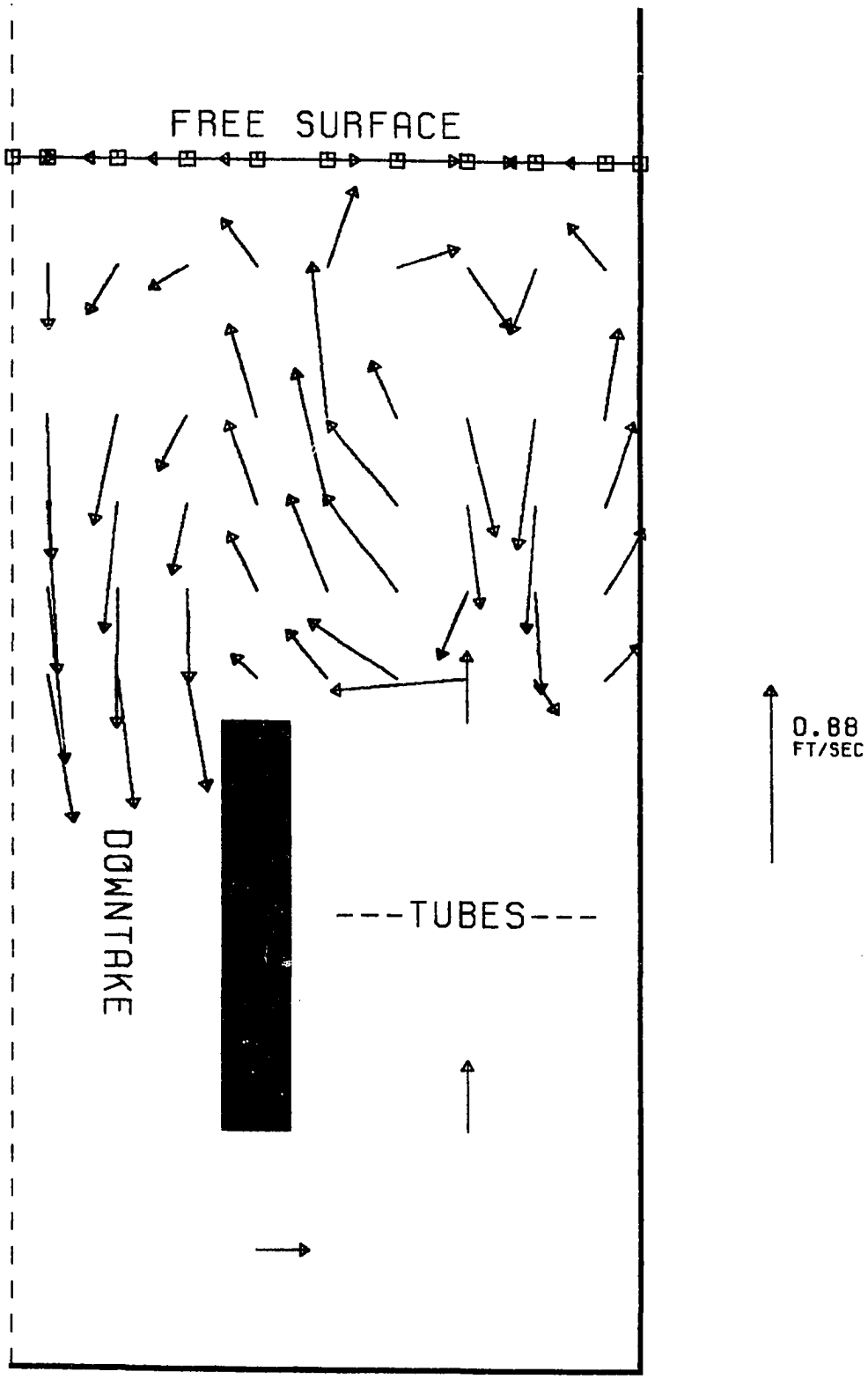
VELOCITY VECTORS

FIGURE II. 2 CASE 2



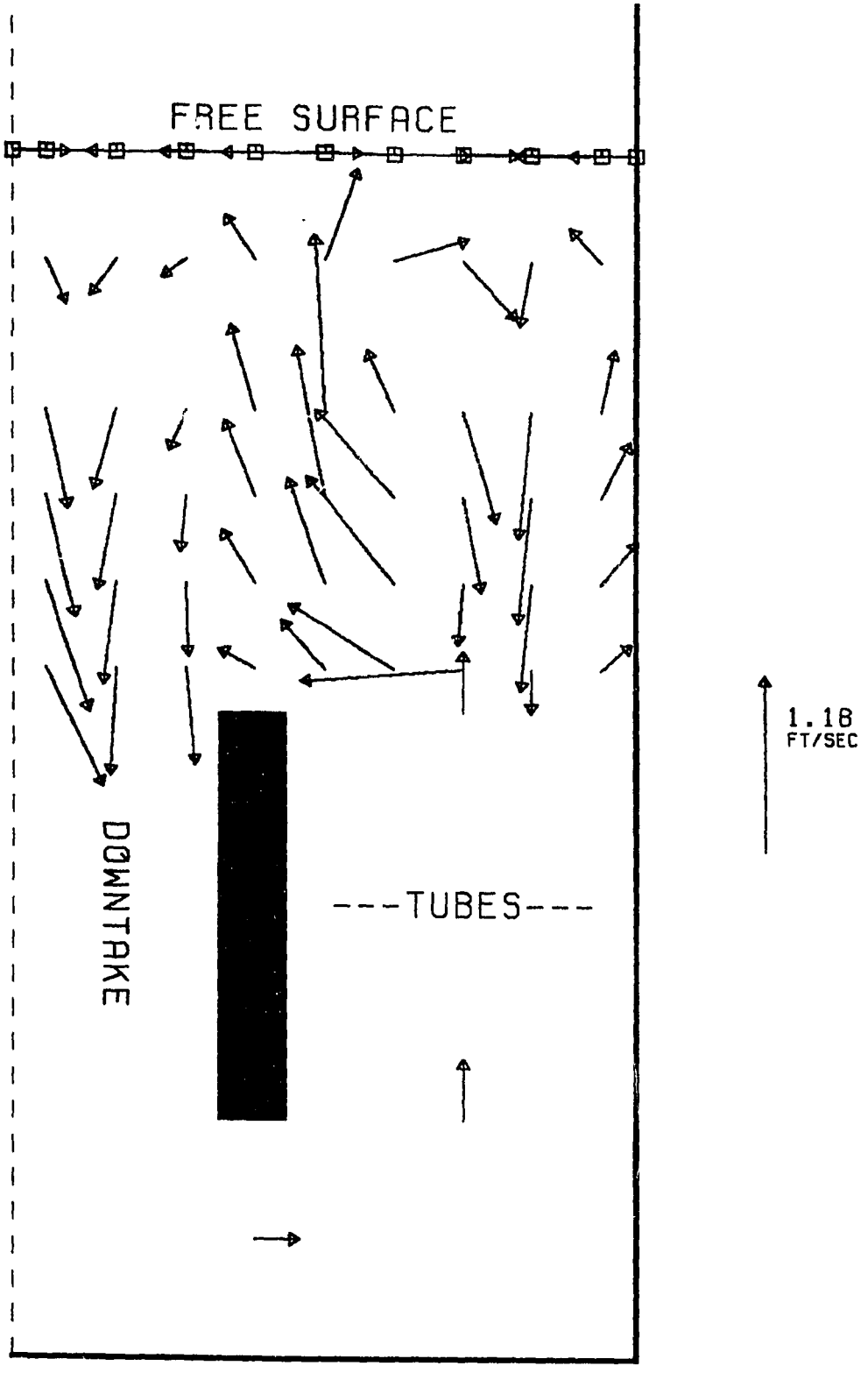
VELOCITY VECTORS

FIGURE II. 3 CASE 3



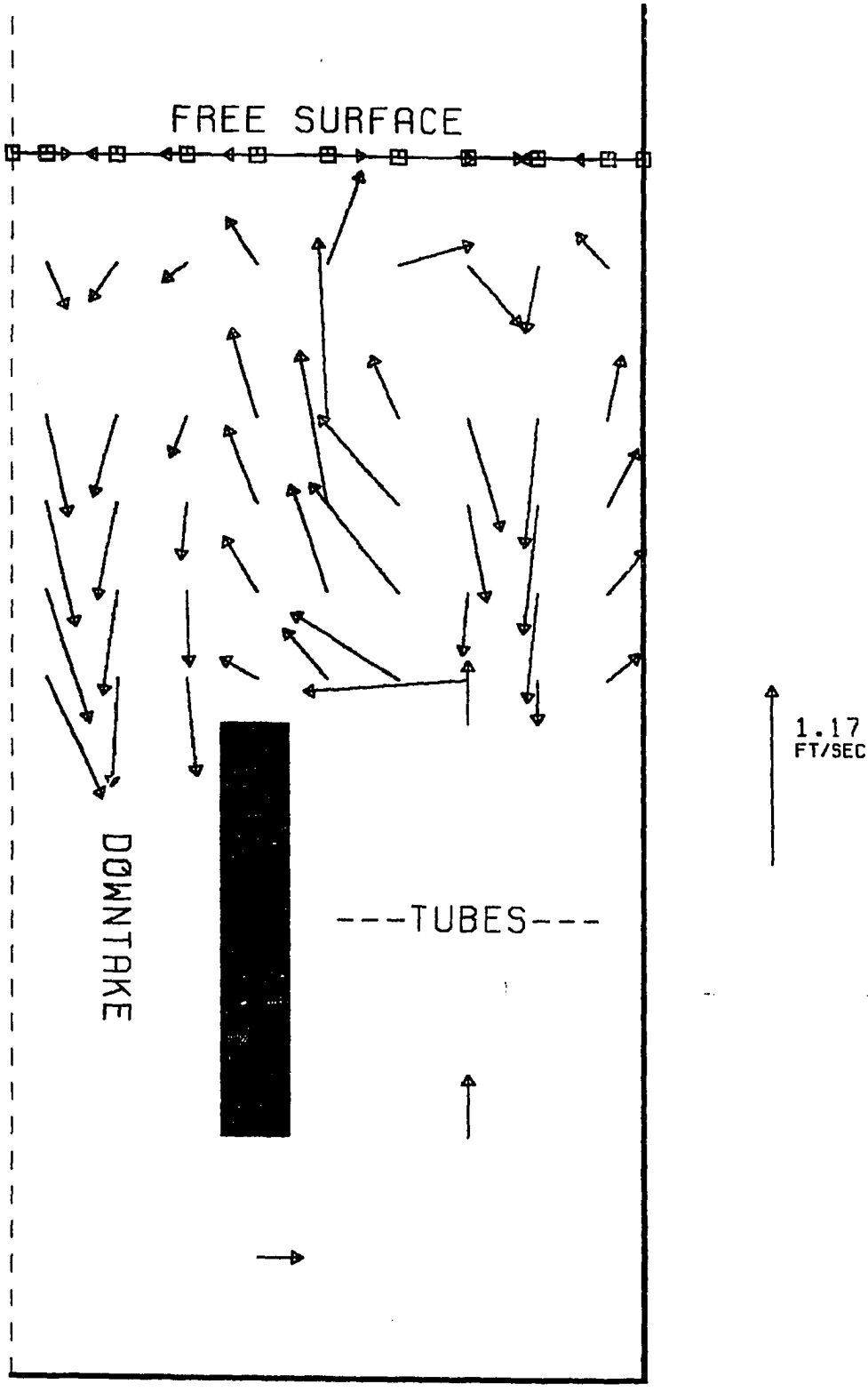
VELOCITY VECTORS

FIGURE II. 4 CASE 4



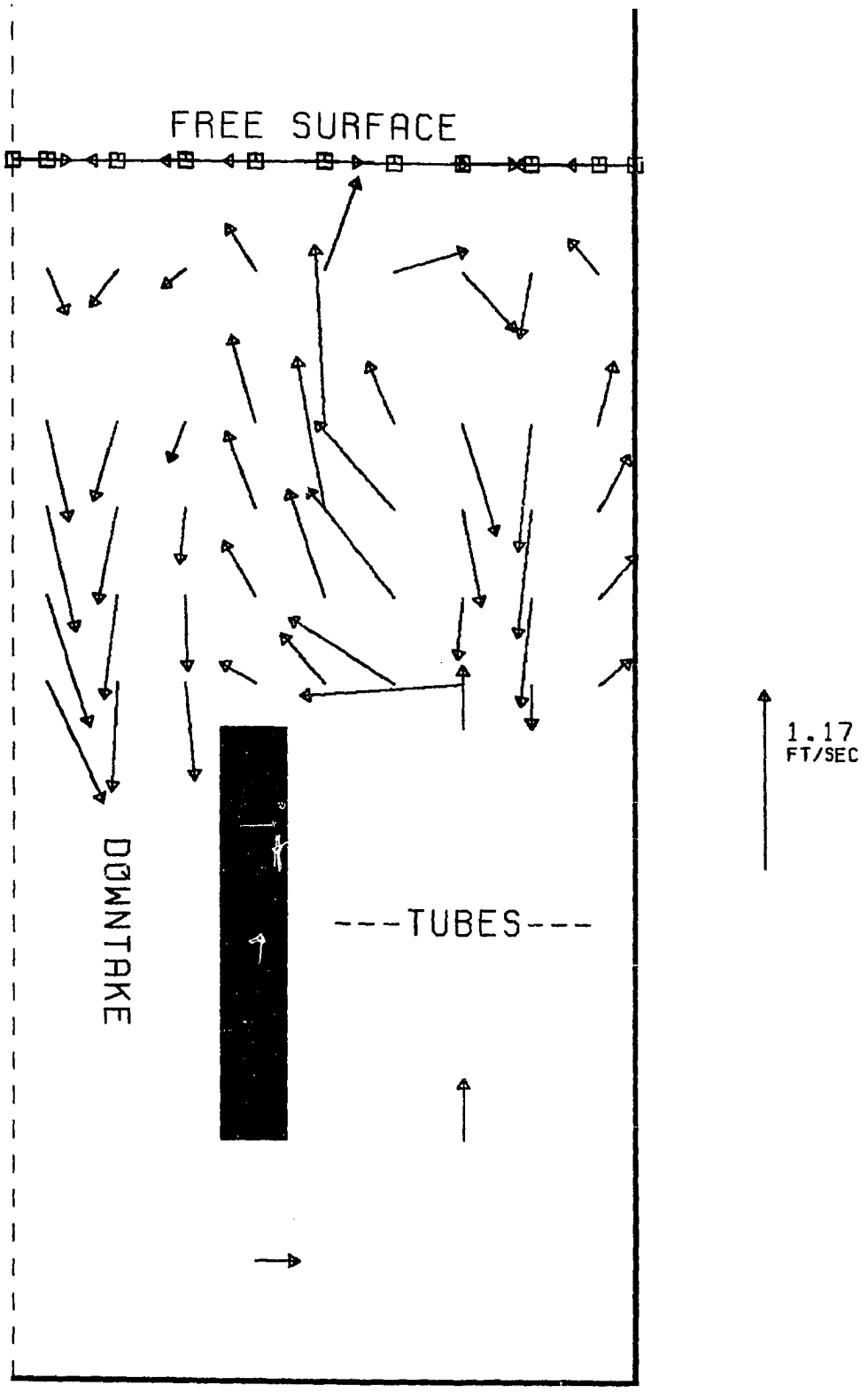
VELOCITY VECTORS

FIGURE II. 5 CASE 5



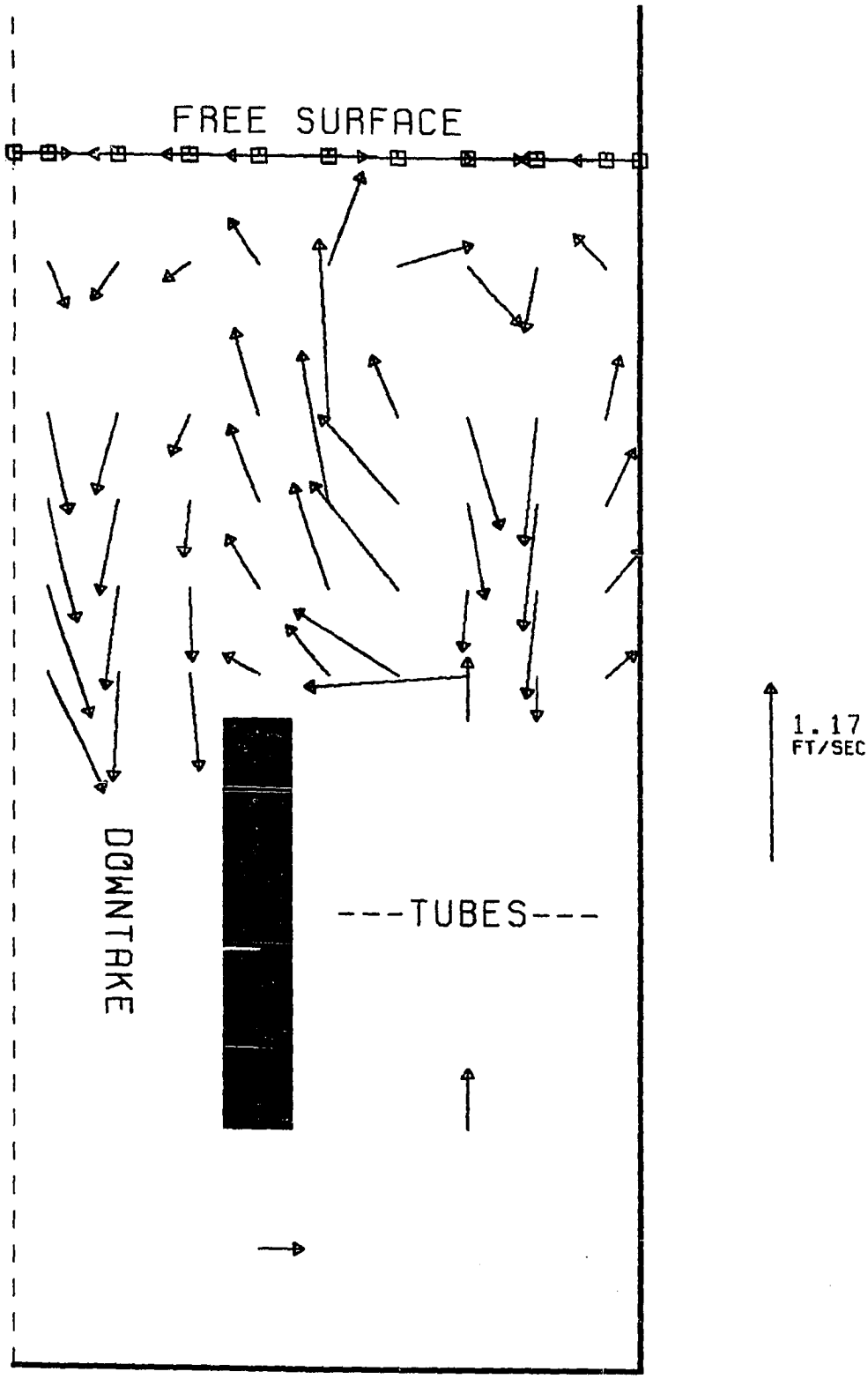
VELOCITY VECTORS

FIGURE II. 6 CASE 6



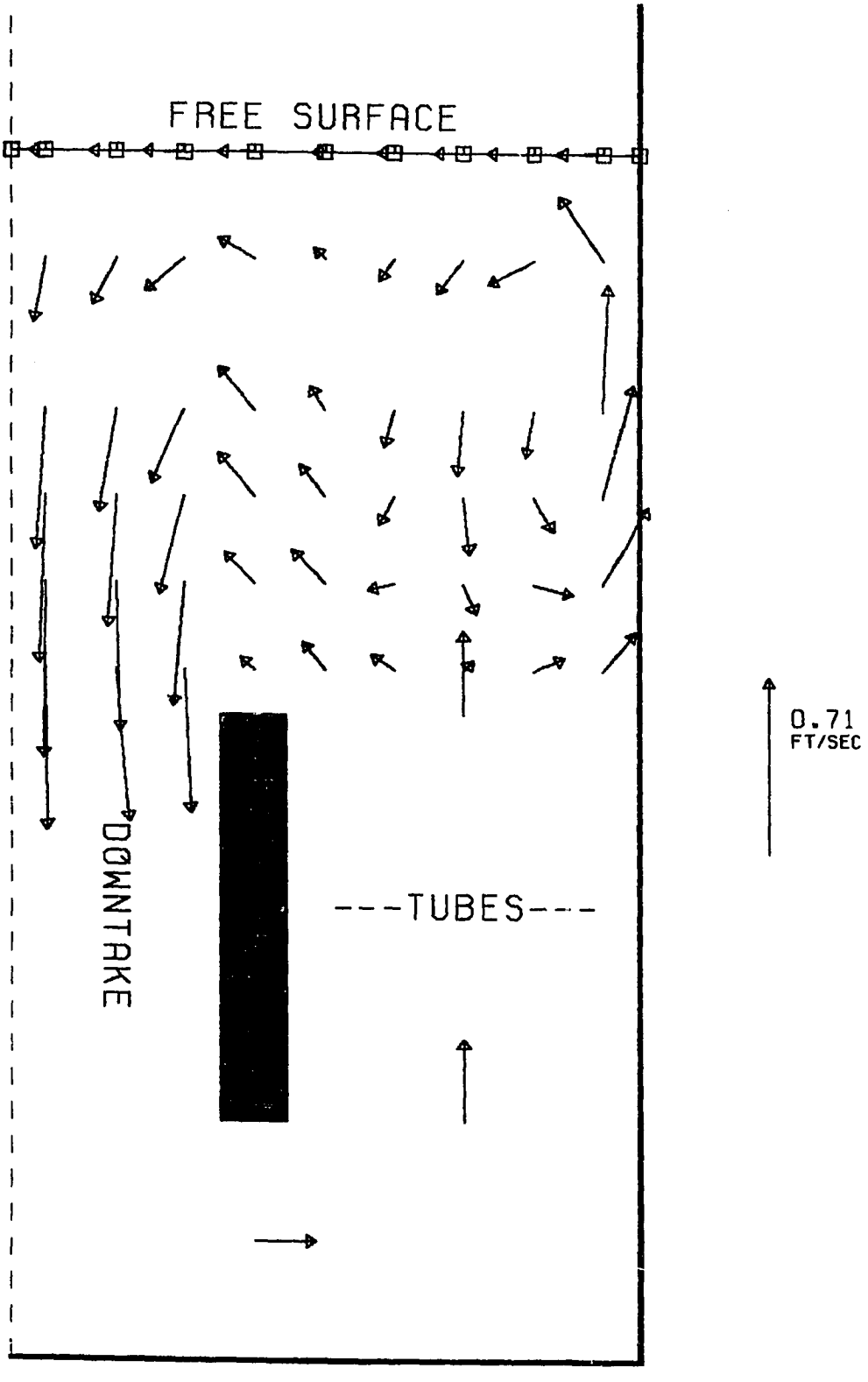
VELOCITY VECTORS

FIGURE II. 7 CASE 7



VELOCITY VECTORS

FIGURE II. 8 CASE 8



VELØCITY VECTØRS

FIGURE II. 9 CASE 9

APPENDIX III

AN EXAMPLE OF DYNAMIC GRID

To demonstrate the dynamic grid, a test case was devised to simulate a typical moving interface under recirculating flow. The test simply consists of adding feed to a partially filled pan while recirculating the fluid in the Pan with a pump. The pump was simulated, as discussed in Chapter 4, by increasing the pressure drop from the Downtake to the Calandria by the amount of pressure head supplied by the pump. The recirculation is then caused by this pressure drop. The Figures III.1-III.3 are snapshots of the Pan at various times. Notice that the tank is filling and the grid formation is expanding in the vertical direction as designed. The total movement of the surface is about one foot. This simple case was devised only because it could be done in a small amount of computer time. A simulation of the Sugar Crystallizer with the same change in volume would take considerably more computer time to demonstrate how the dynamic grid works.

During a simulation of the Crystallizer the grid expands as the volume expands, and contracts when the accumulation of volume in the Pan is negative. This allows the simulation to continue from the beginning of a batch to the end, while the level is changing in

response to crystal growth, feed, and evaporation. Thus, the solution need not be stopped because the surface cell is too large or too small. Although the grid would normally be thought of as moving according to the dynamics of the surface, the movement of the grid can be arbitrary. Thus, with the proper programming, the grid can be made to move at the discretion of the programmer. The dynamic grid is an essential tool for free surface problems.

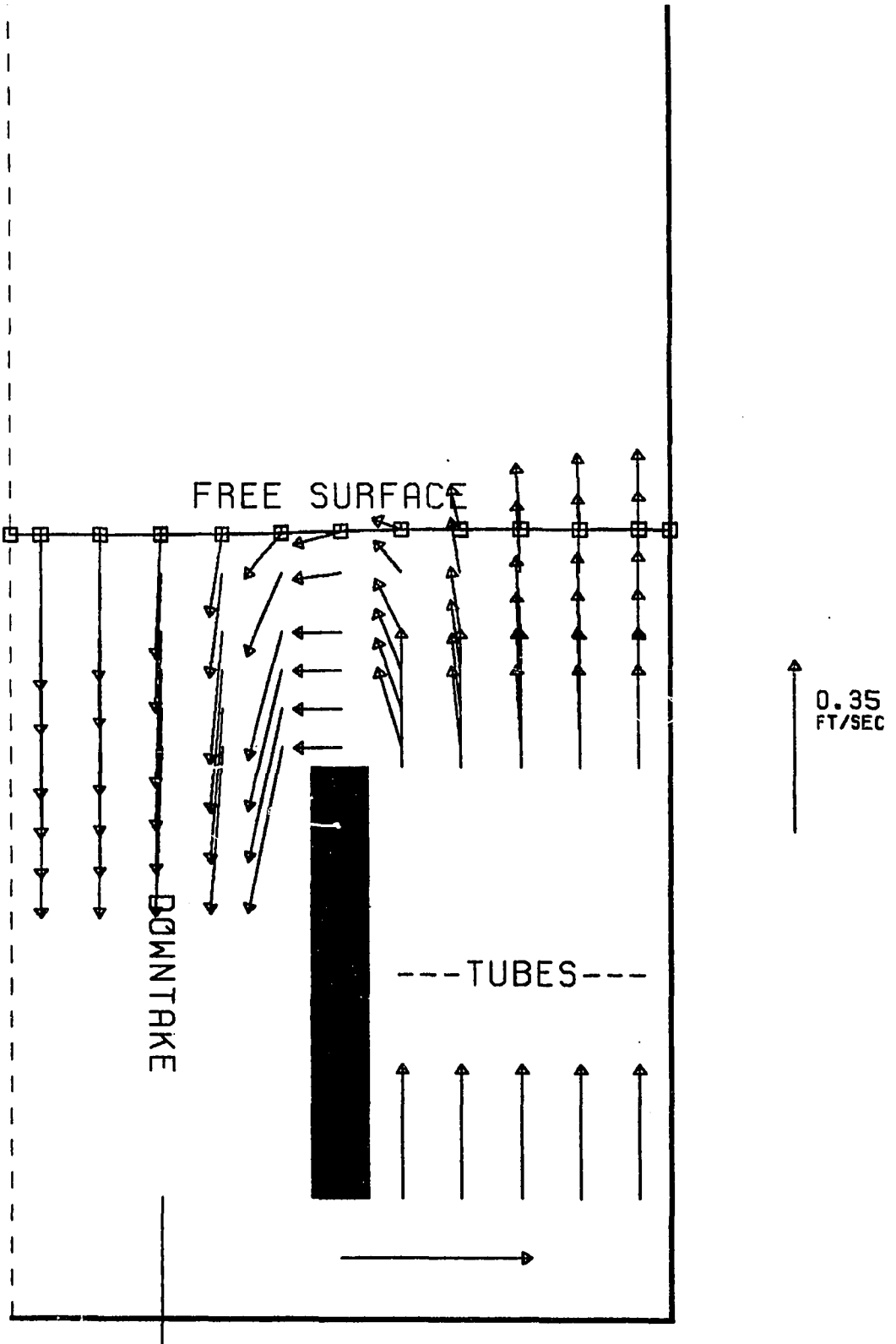
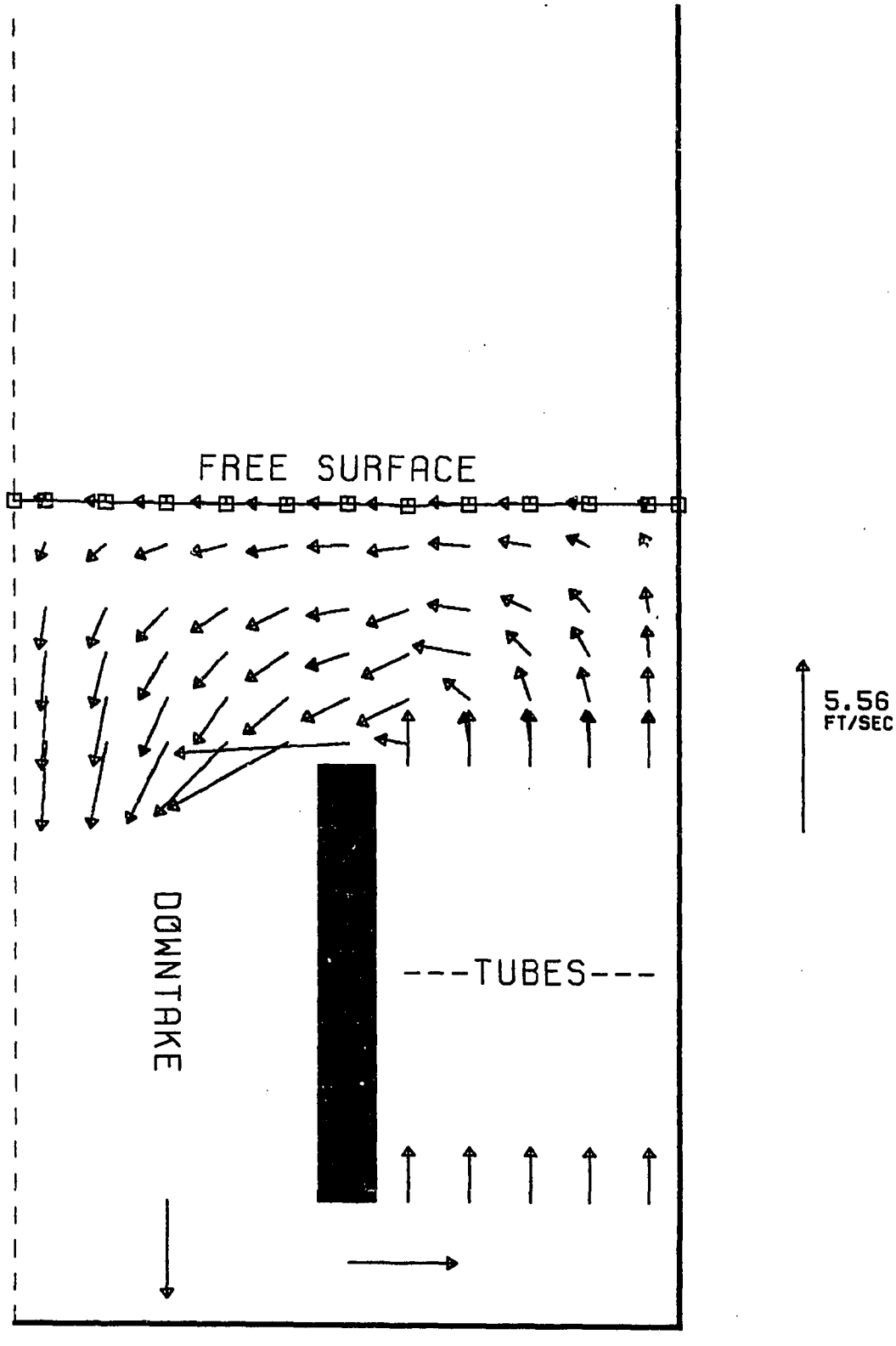
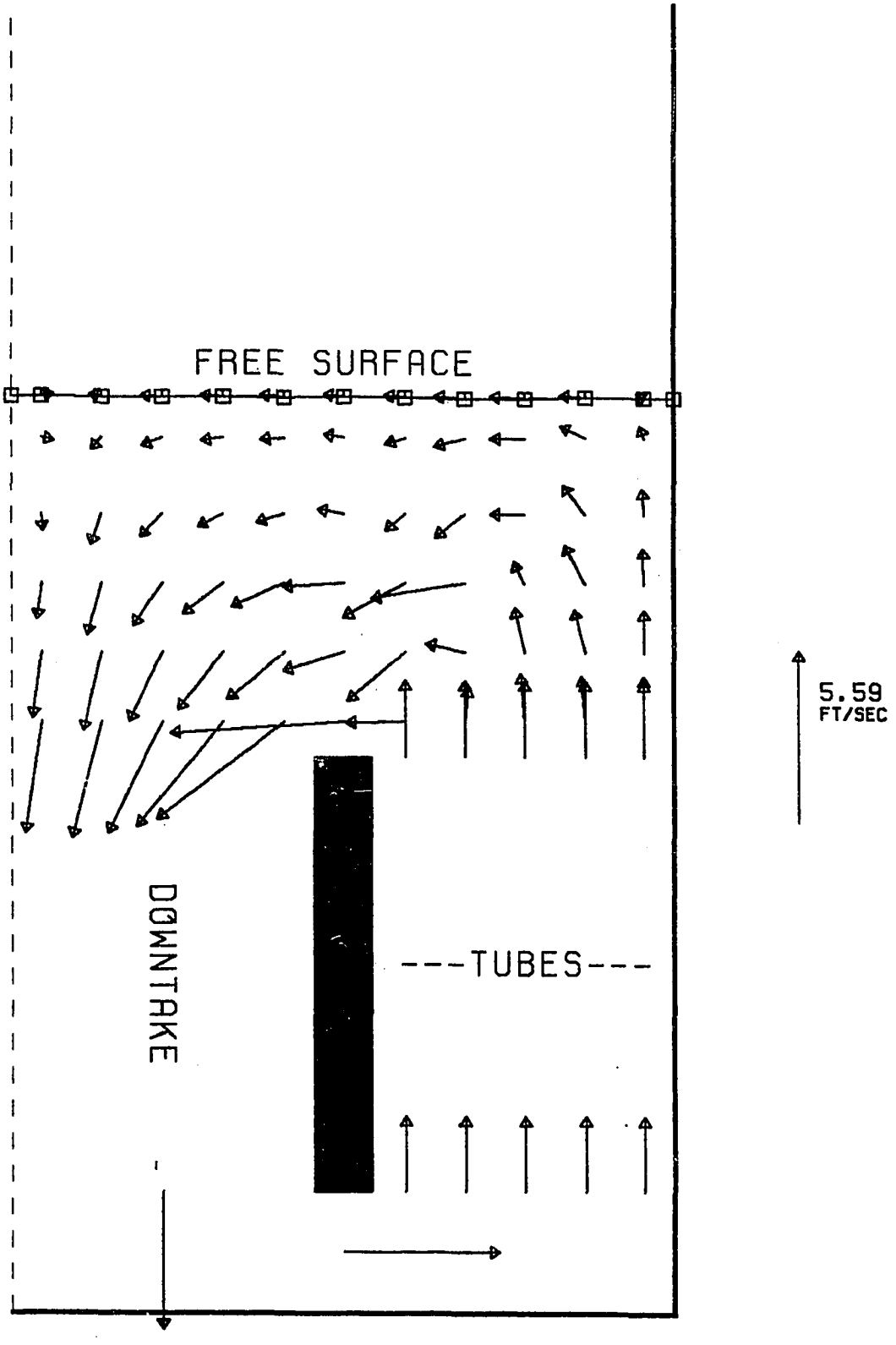


FIGURE III. 1



VELOCITY VECTORS FIGURE III. 2
RUN I.D.:FREE SURFACE
ELAPSED TIME:0.002 HR.



VELOCITY VECTORS FIGURE III. 3
RUN I.D.:FREE SURFACE
ELAPSED TIME:0.008 HR.

VITA

Jack Jerome Bunton was born in Selma, Alabama on the twenty-ninth day of July, 1954. He is the son of Beulah G. Bunton of Mobile, Alabama and the late Oscar F. Bunton, retired United States Air Force T./Sgt. of twenty-three years.

He attended the University of South Alabama following graduation from high school and graduated with a B. S. is Chemical Engineering in 1976. In the Fall of 1976 he entered Graduate School at Louisiana State University and received a M. S. in Chemical Engineering in 1978.

He is married to the former Toni Lynn McLain of Mobile, Alabama. They have a lovely daughter, Brianna. They are presently living in Mobile, Alabama where he is employed by Ciba-Geigy Corp. as a Senior Process Engineer.

EXAMINATION AND THESIS REPORT

Candidate: Jack Jerome Bunton

Major Field: Chemical Engineering

Title of Thesis: Natural Convection, Two-Phase Flow, and Crystallization in a Vacuum Pan Sugar Crystallizer

Approved:

Armando B. Corripio
Major Professor and Chairman

James D. Traynham
Dean of the Graduate School

EXAMINING COMMITTEE:

Ralph W. Pike

Lawrence Mann, Jr.

Joseph A. Polack

Kent Wilkinson

Date of Examination:

November 25, 1980